

## NOUVELLE PROTEINE DE FIXATION DU PHOSPHATE, COMPOSITIONS PHARMACEUTIQUES LA CONTENANT ET SES UTILISATIONS

5 La présente invention a pour objet une nouvelle protéine, issue du sérum humain, de fixation du phosphate, des compositions pharmaceutiques la contenant ainsi que ses utilisations, notamment dans le cadre du traitement de l'hyperphosphatémie et des maladies cardiovasculaires ou de l'arthrite.

10 Le phosphate est une molécule très importante impliquée dans de nombreux mécanismes biologiques. On retrouve notamment le phosphate dans les phospholipides, dans le mécanisme de production d'énergie (ATP, ADP), dans les processus de signalisation cellulaire, dans la composition du matériel génétique dans les os (sous forme de phosphate de calcium).

15 L'hyperphosphatémie est une pathologie liée à un excès de phosphate dans l'organisme et provoque notamment une augmentation des risques de maladies cardiovasculaires, en favorisant les processus d'athérosclérose et de calcification des artères (Dorozhkin et Epple, 2002 ; Amann et al., 2003 ; Blazheevich et al., 1975). La calcification s'effectuant au niveau des articulations, l'hyperphosphatémie peut aussi provoquer de l'arthrite (pseudo-goutte).

20 Les sels de phosphate de calcium produits dans le sérum lors d'une hyperphosphatémie précipitent dans les tissus mous avec calcification ectopique dans différents tissus : vaisseaux (accidents vasculaires cérébraux ou cardiaques), articulations (pseudo-goutte), cristallin, interstitium rénal (néphrocalcinose), sous-cutanées (prurit), pulmonaires, pancréatiques.

25 Ainsi, la moitié des décès chez les personnes souffrant d'insuffisance rénale est due à des maladies cardiovasculaires liées à l'hyperphosphatémie. A cet égard, certains chélateurs du phosphate qui complexent le phosphate dans la lumière intestinale sont actuellement utilisés comme médicament. Cependant, tous ces chélateurs ne sont pas physiologiques. De là découlent certaines complications ou restrictions quant à leur usage.

30 Les préparations contenant du magnésium sont limitées par la survenue de troubles digestifs (diarrhée) et sont à proscrire en raison du risque d'hypermagnésémie. De même, la prescription d'hydroxyde d'aluminium, longtemps utilisé du fait de son efficacité, doit être évitée, ou du moins limitée à de très faibles périodes, en raison du

– ou toute séquence homologue de la séquence SEQ ID NO : 2 ou SEQ ID NO : 3, ayant de préférence une homologie d'au moins environ 80% avec la séquence SEQ ID NO : 2 ou SEQ ID NO : 3, sous réserve que ladite séquence homologue se lie au phosphate,

5 – ou tout fragment d'une des séquences définies ci-dessus, sous réserve que ledit fragment se lie au phosphate, notamment tout fragment étant constitué d'au moins environ 20 acides aminés contigus dans la séquence SEQ ID NO : 2 ou SEQ ID NO : 3.

10 La séquence SEQ ID NO : 2 correspond à la protéine humaine de fixation du phosphate. Cette nouvelle protéine a été isolée dans le plasma humain et sa structure tridimensionnelle montre qu'elle appartient à la classe des "phosphate binding protein" (protéines de fixation du phosphate : PBP). Elle est également appelée par la suite HPBP (protéine humaine de fixation du phosphate).

15 La séquence SEQ ID NO : 3 correspond à une protéine homologue de la protéine de séquence SEQ ID NO : 2, présentant un pourcentage d'identité d'environ 90% avec la séquence SEQ ID NO : 2, et ayant les mêmes propriétés de fixation du phosphate que la séquence SEQ ID NO : 2.

La propriété de fixation du phosphate des séquences de l'invention peut être vérifiée par le test suivant de fixation du phosphate par marquage radioactif :

20 La protéine est fixée sur une membrane de nitrocellulose (dot blot par aspiration). On laisse incuber la membrane dans un tampon radioactif ( $^{32}\text{P}$  (10 mCi/ml, Amersham-Biosciences) 2M ; Tris 50 mM ; pH 8,0)

La membrane est rapidement rincée 2 × 1 min dans un tampon Tris 50 mM, pH 8,0. En exposant un film photographique avec la membrane (environ 45 min) on peut détecter les zones qui fixent le phosphate radioactif (voir Figure 3 ci-après).

25 La présente invention concerne également une séquence nucléotidique codant pour une protéine telle que définie ci-dessus.

La présente invention concerne également un vecteur recombinant, notamment plasmide, cosmide, phage ou ADN de virus, contenant une séquence nucléotidique telle que définie ci-dessus.

30 Selon un mode de réalisation avantageux, la présente invention concerne un vecteur recombinant tel que défini ci-dessus, contenant les éléments nécessaires à l'expression dans une cellule hôte des polypeptides codés par la séquence nucléotidique telle que définie ci-dessus, insérée dans ledit vecteur.

La présente invention concerne plus particulièrement l'utilisation d'une protéine telle que définie ci-dessus, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, dans le cadre de la prévention ou du traitement des maladies cardiovasculaires.

La présente invention concerne également l'utilisation d'une protéine selon l'invention, notamment de la protéine représentée par la séquence SEQ ID NO : 2 ou SEQ ID NO : 3, en association avec une protéine telle qu'un variant de la protéine paraoxonase, dans le cadre de la prophylaxie ou du traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques, tels que le soman, le VX, le tabun ou le sarin, ou dans le cadre du traitement de l'athérosclérose.

La présente invention concerne également un produit de combinaison comprenant au moins une protéine telle que définie ci-dessus, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, et au moins un variant de la protéine paraoxonase, pour une utilisation simultanée, séparée ou étalée dans le temps destiné à la prophylaxie ou au traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques, tels que le soman, le VX, le tabun ou le sarin.

L'utilisation combinée de la protéine de l'invention, notamment SEQ ID NO : 2, avec un variant de la protéine paraoxonase, permet d'accroître la stabilité de la paraoxonase, notamment dans le cadre de la prophylaxie ou du traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques.

La présente invention concerne également une méthode de dosage de la protéine telle que définie ci-dessus, caractérisée en ce qu'elle comprend les étapes suivantes :

– des anticorps monoclonaux de lapin dirigé contre différents épitopes de la protéine de l'invention (anti-HPB) sont fixés sur une plaque et le sérum humain à analyser contenant ladite protéine (HPB) est déposé sur la plaque susmentionnée,

– la plaque est rincée et lavée,

– on dépose sur la plaque des anticorps anti-anticorps de lapin (anti-IGrabbit-per) marqués avec de la peroxydase durant 30 minutes, afin de former un complexe ternaire entre un anticorps monoclinal de lapin, la protéine selon l'invention et un anticorps anti-anticorps de lapin susmentionnés (anti-HPB – HPB – anti-IGrabbit-per),

– la plaque est rincée et lavée,

– on fait réagir la peroxydase fixée sur la plaque avec son substrat (kit disponible en commerce, Chemiluminescent Peroxidase Substrate (Sigma)) et la réaction est arrêtée au bout de 30 minutes avec la 3,3',5,5'-tétraméthylbenzidine (TMB, Sigma),

plaques d'athéromes, ou au diagnostic *in vitro* d'une prédisposition d'un individu au développement d'une des maladies susmentionnées.

La présente invention concerne également l'application telle que définie ci-dessus au diagnostic *in vitro* de maladies liées à une hypophosphatémie, ou au diagnostic *in vitro* d'une prédisposition d'un individu au développement de ces maladies.

5 Parmi les signes cliniques ou physiologiques caractérisant les maladies liées à une hypophosphatémie, on peut citer :

- une déminéralisation des os,
- les manifestations musculaires de l'hypophosphatémie qui comportent une myopathie proximale affectant le muscle squelettique et une dysphagie et un iléus affectant les muscles lisses,
- des carences cardiopulmonaires par le manque d'ATP, et
- une encéphalopathie métabolique.

## PARTIE EXPÉIMENTALE

### Isolation de la protéine

La protéine SEQ ID NO : 2 est obtenue à partir du plasma humain selon le 5 procédé de Gan et al. (1991) suivant :

La protéine SEQ ID NO : 2 est purifiée à partir de poches de plasma congelé (~200 ml) fournies par l'Etablissement de Transfusion Sanguine de Lyon-Beynost. Le caillot de fibrine, formé par l'ajout de 1 M (1% v/v) de CaCl<sub>2</sub> au plasma est séparé du 10 sérum par filtration. Le sérum est alors mélangé à 400 ml de Gel d'affinité (Cibacron 3GA-Agarose, C-1535, Sigma) équilibré avec un tampon A (Tris/HCl 50 mM, CaCl<sub>2</sub> 1mM, NaCl 4M, pH 8). Dans ces conditions, principalement les HDL ("high density lipoprotein" : lipoprotéines de haute densité) sont adsorbées. Après 6 à 8 heures 15 d'incubation, les protéines non adsorbées sur le gel sont éliminées par filtration sur fritté de porosité n°2. Ce lavage s'effectue jusqu'à ce que l'on ne détecte plus de protéine dans l'éluat (absorption UV à 280 nm). Le gel est ensuite équilibré avec un tampon B (Tris/HCl 50 mM, CaCl<sub>2</sub> 1mM, pH 8) puis placé en colonne XK 50/30 (Pharmacia). L'élution est réalisée en rajoutant 1g/l de déoxycholate de sodium et 0,1% de triton X- 20 100 au tampon B. Les fractions montrant une activité arylestérase sont injectées sur 50 ml d'un gel échangeur d'anions (DEAE Sepharose Fast Flow, Pharmacia) disposé en colonne XK 26/70 (Pharmacia) et équilibré avec le tampon B et 0,05% de triton X-100. L'élution se fait par gradient de NaCl. Un premier palier est réalisé à 87,5 mM de NaCl 25 afin d'éliminer l'apo A-I, une protéine liée à la paraoxonase, et la majorité des protéines contaminantes. La paraoxonase humaine (PON1) est environ éluée à la concentration de 140 mM de NaCl. Toutes les fractions conservées montrent une activité paraoxonase et arylestérase, ces activités étant vérifiées selon les tests mentionnés plus loin. Les fractions éluées ne sont pas regroupées. Les gels SDS-PAGE des fractions obtenues montrent des bandes comprises entre 38 kDa et 45 kDa (voir Figure 1). Chaque purification n'apporte pas toujours la même distribution de masse apparente. Cette 30 légère hétérogénéité peut s'expliquer par la présence de 2 chaînes glycosylées sur la PON1.

En plus de la PON1 dans ces lots une autre protéine a été isolée par cristallisation, en substituant le triton par le C12-maltoside et en utilisant le sulfate d'ammonium comme agent précipitant. Les cristaux obtenus sont ceux d'une protéine inconnue caractérisée par radiocristallographie et correspondant à la séquence SEQ ID NO : 2 de

En raison de la très bonne qualité des cartes de densité électronique, la séquence primaire de la protéine a pu être assignée avec 80% de fiabilité. Une molécule de phosphate a aussi pu être localisée.

La structure obtenue ne correspond pas du tout à la paraoxonase humaine. Le séquençage obtenu en identifiant les acides aminés à partir de la densité électronique indique que ni cette protéine humaine ni son gène n'ont été décrits auparavant. Il s'agit donc d'une nouvelle protéine.

La structure de la protéine de l'invention montre une très forte homologie avec la protéine de fixation du phosphate ("phosphate binding") d'*Escherichia coli*. Cette protéine chez cette bactérie sert à transporter le phosphate à travers le périplasme. On la retrouve chez beaucoup de procaryotes mais chez aucun eucaryote.

La densité électronique a aussi montré qu'une molécule de phosphate était fixée à la nouvelle protéine de l'invention, de la même façon que dans celle d'*Escherichia coli*.

Ainsi, on peut conclure que la protéine de l'invention caractérisée à partir du plasma humain présente une très forte homologie avec la protéine bactérienne et qu'elle est capable de fixer le phosphate et de le transporter.

### Séquençage

#### *Digestion dans le gel*

Le mélange paraoxonase-HPBP a été séparé par gel électrophorétique avec SDS-PAGE (sans chauffage). Plusieurs bandes correspondant à HPBP aux alentour de 70 kDa ont été découpées.

La digestion de la protéine contenue dans ces bandes a été effectuée grâce au système automatique de digestion, MassPrep Sation (Waters Manchester, G.B.). Les bandes de gel ont été lavées deux fois avec 50 µl d'une solution à 25 mM de carbonate d'ammonium hydrogéné (NH<sub>4</sub>HCO<sub>3</sub>) et 50 µl d'acétonitrile. Les cystéines ont été réduites avec 50 µl d'une solution à 10mM de dithiothréitol à 57°C et acylé avec 50 µl de iodocacétamide à 55 mM. Après déshydratation avec l'acétonitrile, la protéine a été digérée enzymatiquement avec 10 µl de trypsine porcine modifiée à 12,5 ng/µl (Promega, Madisson, WI, U.S.A) ou bien avec lys-C de Lysobacter enzymogenes (Roche Applied Science, Penzberg, Germany) dans 25 mM de NH<sub>4</sub>HCO<sub>3</sub>. La digestion s'est opérée une nuit complète à température ambiante. Les peptides clivés ont été extraits avec une solution à 60% d'acétonitrile et 5% d'acide formique.

L'acquisition des données de masse a été pilotée par le programme MassLynx (Micromass, Manchester, G.B.) qui bascule automatiquement entre le mode MS et le mode MS/MS.

Les spectres MS/MS générés ont été individuellement séquencés *de novo* afin d'obtenir la séquence partielle ou complète. Ces interprétations ont été réalisées en utilisant le programme PepSeq (MassLynx, Micromass) et le programme PEAKS Studio (Bioinformatics Solutions, Waterloo, Canada) qui sont capables de traiter complètement un fichier .pkl avec un séquençage *de novo* automatique sur chaque spectre MS/MS.

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#### Fixation du phosphate

La fixation du phosphate par la protéine de l'invention SEQ ID NO : 2 a été mise en évidence selon le test suivant :

On dépose 200 µl de la protéine de l'invention SEQ ID NO : 2 (colonnes A-F de la Figure 3), ou du lysozyme 1 mg/ml (colonne G) ou de la βlacto-globuline sur nitrocellulose (dot blot par aspiration).

L'ensemble est incubé pendant 2 h 30 dans un mélange comprenant : tris 50 mM ; pH 8,0 ;  $^{32}\text{P}$  (10 mCi/ml) 2 mM.

On effectue ensuite un rinçage 2 fois pendant 1 minute avec du tris 50 mM à pH 8,0, puis on expose l'ensemble à température ambiante pendant 45 minutes.

On constate alors (voir Figure 3) que la protéine de l'invention a fixé le phosphate radioactif (colonnes A à F), alors que les témoins tests ne l'ont pas fixée (colonnes G et H).

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#### Rôle et utilisation de la protéine SEQ ID NO : 2

Pour doser la concentration de cette protéine dans le plasma les méthodes utilisables sont :

- les méthodes électrophorétiques,
- la purification de la protéine,
- la quantification de son activité,
- l'immunodosage de la protéine en utilisant des anticorps polyclonaux/monoclonaux dirigé contre la protéine.

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5. Vecteur recombinant selon la revendication 4, contenant les éléments nécessaires à l'expression dans une cellule hôte des polypeptides codés par une séquence nucléotidique selon la revendication 3, insérés dans ledit vecteur.

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6. Cellule hôte, choisie notamment parmi les bactéries, les levures, les cellules de champignons, les cellules de plantes ou les cellules de mammifères, ladite cellule hôte étant transformée à l'aide d'un vecteur recombinant selon l'une des revendications 4 ou 5.

10

7. Composition pharmaceutique comprenant à titre de substance active une protéine selon la revendication 1 ou 2, en association avec un véhicule pharmaceutiquement acceptable.

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8. Composition pharmaceutique selon la revendication 7, comprenant à titre de substance active une protéine représentée par la séquence SEQ ID NO : 2 ou SEQ ID NO : 3.

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9. Composition pharmaceutique selon la revendication 8, dans laquelle la protéine telle que définie dans la revendication 1 ou 2, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, est en association avec un variant de la protéine paraoxonase, notamment SEQ ID NO : 4, SEQ ID NO : 5, SEQ ID NO : 6, SEQ ID NO : 7, SEQ ID NO : 8, SEQ ID NO : 9, SEQ ID NO : 10 ou SEQ ID NO : 11.

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10. Utilisation d'une protéine selon la revendication 1 ou 2, notamment de la protéine représentée par la séquence SEQ ID NO : 2 ou SEQ ID NO : 3, pour la préparation d'un médicament destiné à la prévention ou au traitement de l'arthrite ou de maladies liées à une hyperphosphatémie, telles que les maladies cardiovasculaires, ou, en association avec un variant de la protéine paraoxonase, notamment SEQ ID NO : 4, SEQ ID NO : 5, SEQ ID NO : 6, SEQ ID NO : 7, SEQ ID NO : 8, SEQ ID NO : 9, SEQ ID NO : 10 ou SEQ ID NO : 11, dans le cadre de la prophylaxie ou du traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques tels que le soman, le VX, le sarin ou le tabun, ou dans le cadre du traitement de l'athérosclérose.

30

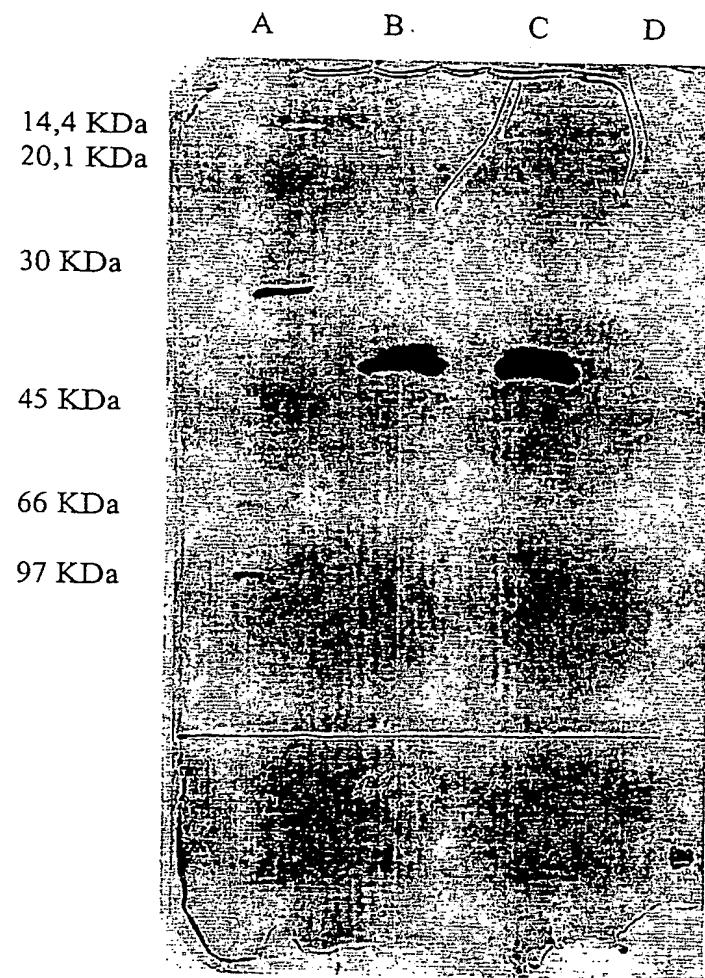
au diagnostic *in vitro* de maladies liées à une hypophosphatémie notamment lorsque la quantité de protéine selon la revendication 1 ou 2, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, dosée selon la méthode de la revendication 12, est supérieure à la quantité de cette protéine normalement présente dans le sang d'un individu sain, ou

5 au diagnostic *in vitro* d'une prédisposition d'un individu à de telles pathologies.

10 14. Application selon la revendication 13 au diagnostic *in vitro* de maladies liées à une hyperphosphatémie telles que les maladies cardiovasculaires, notamment les maladies cardiovasculaires liées à la formation de plaques d'athéromes, ou au diagnostic *in vitro* d'une prédisposition d'un individu au développement d'une des maladies susmentionnées.

15 15. Application selon la revendication 14 au diagnostic *in vitro* de maladies liées à une hypophosphatémie, ou au diagnostic *in vitro* d'une prédisposition d'un individu au développement de ces maladies.

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**FIGURE 1**

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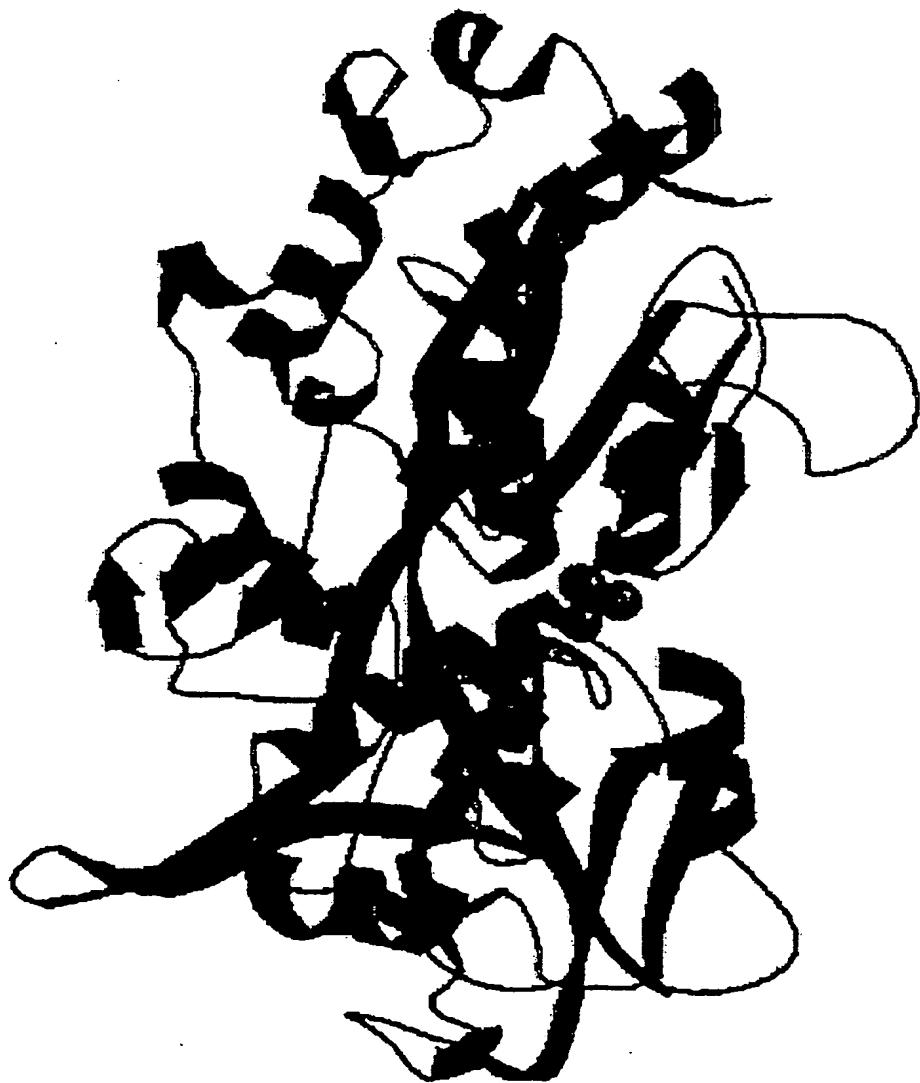
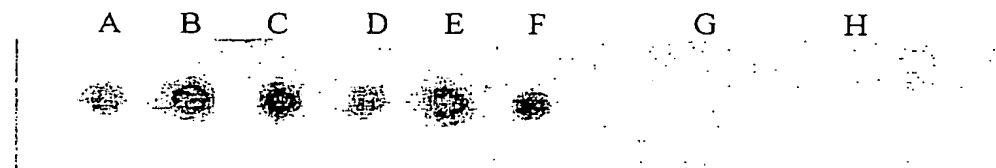


FIGURE 2

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**FIGURE 3**

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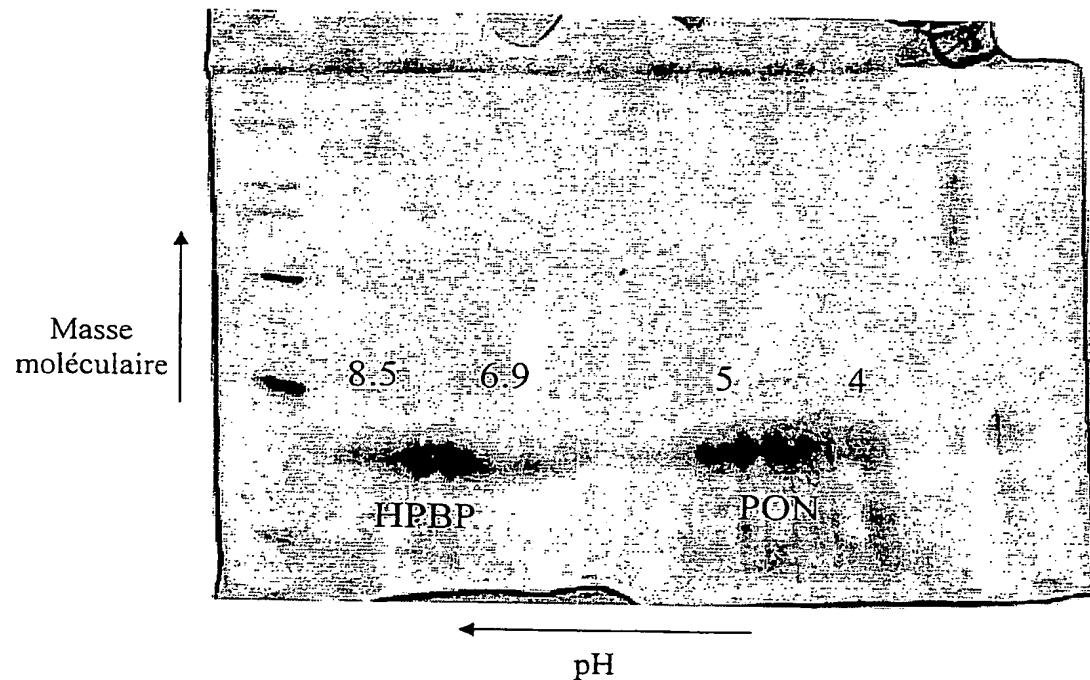


FIGURE 4

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|      |    |     |     |   |    |        |        |        |      |       |   |
|------|----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 1  | CB  | SER | A | 1  | 24.666 | 45.653 | 14.370 | 1.00 | 26.15 | A |
| ATOM | 2  | OG  | SER | A | 1  | 25.258 | 46.028 | 13.130 | 1.00 | 38.82 | A |
| ATOM | 3  | C   | SER | A | 1  | 22.519 | 45.324 | 15.622 | 1.00 | 20.30 | A |
| ATOM | 4  | O   | SER | A | 1  | 21.889 | 46.093 | 16.367 | 1.00 | 18.83 | A |
| ATOM | 5  | N   | SER | A | 1  | 22.817 | 47.273 | 14.074 | 1.00 | 22.37 | A |
| ATOM | 6  | CA  | SER | A | 1  | 23.146 | 45.831 | 14.317 | 1.00 | 22.87 | A |
| ATOM | 7  | N   | ILE | A | 2  | 22.676 | 44.027 | 15.878 | 1.00 | 14.00 | A |
| ATOM | 8  | CA  | ILE | A | 2  | 22.149 | 43.401 | 17.092 | 1.00 | 13.36 | A |
| ATOM | 9  | CB  | ILE | A | 2  | 21.747 | 41.923 | 16.828 | 1.00 | 14.04 | A |
| ATOM | 10 | CG2 | ILE | A | 2  | 21.536 | 41.191 | 18.155 | 1.00 | 9.05  | A |
| ATOM | 11 | CG1 | ILE | A | 2  | 20.458 | 41.872 | 15.988 | 1.00 | 13.38 | A |
| ATOM | 12 | CD1 | ILE | A | 2  | 20.173 | 40.501 | 15.357 | 1.00 | 14.27 | A |
| ATOM | 13 | C   | ILE | A | 2  | 23.303 | 43.459 | 18.083 | 1.00 | 12.32 | A |
| ATOM | 14 | O   | ILE | A | 2  | 24.376 | 42.890 | 17.847 | 1.00 | 14.26 | A |
| ATOM | 15 | N   | ASP | A | 3  | 23.075 | 44.122 | 19.205 | 1.00 | 13.19 | A |
| ATOM | 16 | CA  | ASP | A | 3  | 24.134 | 44.331 | 20.193 | 1.00 | 11.15 | A |
| ATOM | 17 | CB  | ASP | A | 3  | 24.149 | 45.830 | 20.578 | 1.00 | 12.52 | A |
| ATOM | 18 | CG  | ASP | A | 3  | 24.268 | 46.744 | 19.351 | 1.00 | 11.70 | A |
| ATOM | 19 | OD1 | ASP | A | 3  | 25.289 | 46.618 | 18.642 | 1.00 | 11.97 | A |
| ATOM | 20 | OD2 | ASP | A | 3  | 23.356 | 47.569 | 19.094 | 1.00 | 13.82 | A |
| ATOM | 21 | C   | ASP | A | 3  | 23.981 | 43.508 | 21.456 | 1.00 | 11.88 | A |
| ATOM | 22 | O   | ASP | A | 3  | 22.947 | 43.577 | 22.116 | 1.00 | 11.48 | A |
| ATOM | 23 | N   | GLY | A | 4  | 25.022 | 42.763 | 21.800 | 1.00 | 9.46  | A |
| ATOM | 24 | CA  | GLY | A | 4  | 24.973 | 41.947 | 23.007 | 1.00 | 10.97 | A |
| ATOM | 25 | C   | GLY | A | 4  | 26.303 | 41.966 | 23.740 | 1.00 | 8.48  | A |
| ATOM | 26 | O   | GLY | A | 4  | 27.314 | 42.413 | 23.200 | 1.00 | 9.87  | A |
| ATOM | 27 | N   | GLY | A | 5  | 26.296 | 41.496 | 24.987 | 1.00 | 11.77 | A |
| ATOM | 28 | CA  | GLY | A | 5  | 27.511 | 41.489 | 25.785 | 1.00 | 4.85  | A |
| ATOM | 29 | C   | GLY | A | 5  | 27.163 | 41.000 | 27.186 | 1.00 | 8.06  | A |
| ATOM | 30 | O   | GLY | A | 5  | 26.009 | 40.610 | 27.447 | 1.00 | 9.13  | A |
| ATOM | 31 | N   | GLY | A | 6  | 28.144 | 41.021 | 28.089 | 1.00 | 9.80  | A |
| ATOM | 32 | CA  | GLY | A | 6  | 27.898 | 40.589 | 29.458 | 1.00 | 9.86  | A |
| ATOM | 33 | C   | GLY | A | 6  | 28.970 | 39.679 | 30.014 | 1.00 | 7.11  | A |
| ATOM | 34 | O   | GLY | A | 6  | 30.150 | 40.030 | 30.000 | 1.00 | 8.89  | A |
| ATOM | 35 | N   | ALA | A | 7  | 28.567 | 38.518 | 30.525 | 1.00 | 9.08  | A |
| ATOM | 36 | CA  | ALA | A | 7  | 29.509 | 37.540 | 31.079 | 1.00 | 8.69  | A |
| ATOM | 37 | CB  | ALA | A | 7  | 28.814 | 36.168 | 31.195 | 1.00 | 7.94  | A |
| ATOM | 38 | C   | ALA | A | 7  | 30.811 | 37.363 | 30.277 | 1.00 | 9.69  | A |
| ATOM | 39 | O   | ALA | A | 7  | 30.781 | 37.212 | 29.050 | 1.00 | 7.30  | A |
| ATOM | 40 | N   | THR | A | 8  | 31.941 | 37.367 | 30.981 | 1.00 | 7.56  | A |
| ATOM | 41 | CA  | THR | A | 8  | 33.236 | 37.135 | 30.338 | 1.00 | 7.21  | A |
| ATOM | 42 | CB  | THR | A | 8  | 34.402 | 37.865 | 31.065 | 1.00 | 8.00  | A |
| ATOM | 43 | OG1 | THR | A | 8  | 34.532 | 37.344 | 32.402 | 1.00 | 9.83  | A |
| ATOM | 44 | CG2 | THR | A | 8  | 34.123 | 39.388 | 31.139 | 1.00 | 10.68 | A |
| ATOM | 45 | C   | THR | A | 8  | 33.542 | 35.624 | 30.340 | 1.00 | 5.67  | A |
| ATOM | 46 | O   | THR | A | 8  | 34.355 | 35.168 | 29.552 | 1.00 | 8.00  | A |
| ATOM | 47 | N   | LEU | A | 9  | 32.885 | 34.842 | 31.195 | 1.00 | 6.65  | A |
| ATOM | 48 | CA  | LEU | A | 9  | 33.190 | 33.389 | 31.224 | 1.00 | 9.98  | A |
| ATOM | 49 | CB  | LEU | A | 9  | 32.275 | 32.649 | 32.238 | 1.00 | 10.55 | A |
| ATOM | 50 | CG  | LEU | A | 9  | 32.400 | 31.109 | 32.271 | 1.00 | 11.53 | A |
| ATOM | 51 | CD1 | LEU | A | 9  | 32.200 | 30.566 | 33.699 | 1.00 | 10.77 | A |
| ATOM | 52 | CD2 | LEU | A | 9  | 31.356 | 30.503 | 31.300 | 1.00 | 6.94  | A |
| ATOM | 53 | C   | LEU | A | 9  | 33.103 | 32.755 | 29.817 | 1.00 | 10.91 | A |
| ATOM | 54 | O   | LEU | A | 9  | 33.985 | 31.970 | 29.421 | 1.00 | 9.67  | A |
| ATOM | 55 | N   | PRO | A | 10 | 32.051 | 33.088 | 29.040 | 1.00 | 6.59  | A |
| ATOM | 56 | CD  | PRO | A | 10 | 30.763 | 33.664 | 29.485 | 1.00 | 8.09  | A |
| ATOM | 57 | CA  | PRO | A | 10 | 31.915 | 32.521 | 27.686 | 1.00 | 7.68  | A |
| ATOM | 58 | CB  | PRO | A | 10 | 30.428 | 32.218 | 27.611 | 1.00 | 11.73 | A |
| ATOM | 59 | CG  | PRO | A | 10 | 29.845 | 33.467 | 28.251 | 1.00 | 8.40  | A |
| ATOM | 60 | C   | PRO | A | 10 | 32.317 | 33.504 | 26.579 | 1.00 | 8.72  | A |
| ATOM | 61 | O   | PRO | A | 10 | 32.040 | 33.263 | 25.396 | 1.00 | 9.01  | A |
| ATOM | 62 | N   | GLU | A | 11 | 33.003 | 34.589 | 26.928 | 1.00 | 5.35  | A |
| ATOM | 63 | CA  | GLU | A | 11 | 33.325 | 35.565 | 25.896 | 1.00 | 8.04  | A |
| ATOM | 64 | CB  | GLU | A | 11 | 33.978 | 36.829 | 26.493 | 1.00 | 12.60 | A |
| ATOM | 65 | CG  | GLU | A | 11 | 35.380 | 36.672 | 27.001 | 1.00 | 21.32 | A |
| ATOM | 66 | CD  | GLU | A | 11 | 35.994 | 38.013 | 27.391 | 1.00 | 26.61 | A |
| ATOM | 67 | OE1 | GLU | A | 11 | 35.264 | 38.873 | 27.920 | 1.00 | 30.93 | A |
| ATOM | 68 | OE2 | GLU | A | 11 | 37.203 | 38.202 | 27.176 | 1.00 | 31.32 | A |
| ATOM | 69 | C   | GLU | A | 11 | 34.143 | 35.066 | 24.709 | 1.00 | 10.00 | A |
| ATOM | 70 | O   | GLU | A | 11 | 33.866 | 35.464 | 23.563 | 1.00 | 8.68  | A |
| ATOM | 71 | N   | LYS | A | 12 | 35.134 | 34.215 | 24.957 | 1.00 | 8.65  | A |
| ATOM | 72 | CA  | LYS | A | 12 | 35.935 | 33.678 | 23.850 | 1.00 | 10.43 | A |
| ATOM | 73 | CB  | LYS | A | 12 | 37.081 | 32.840 | 24.374 | 1.00 | 11.05 | A |
| ATOM | 74 | CG  | LYS | A | 12 | 38.151 | 33.646 | 25.090 | 1.00 | 9.26  | A |
| ATOM | 75 | CD  | LYS | A | 12 | 39.117 | 32.622 | 25.673 | 1.00 | 17.64 | A |

FIGURE 5

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 76  | CE  | LYS | A | 12 | 40.293 | 33.277 | 26.307 | 1.00 | 24.93 | A |
| ATOM | 77  | NZ  | LYS | A | 12 | 41.298 | 32.237 | 26.600 | 1.00 | 25.96 | A |
| ATOM | 78  | C   | LYS | A | 12 | 35.079 | 32.830 | 22.934 | 1.00 | 11.17 | A |
| ATOM | 79  | O   | LYS | A | 12 | 35.339 | 32.726 | 21.736 | 1.00 | 8.79  | A |
| ATOM | 80  | N   | LEU | A | 13 | 34.071 | 32.176 | 23.498 | 1.00 | 7.67  | A |
| ATOM | 81  | CA  | LEU | A | 13 | 33.189 | 31.383 | 22.669 | 1.00 | 10.04 | A |
| ATOM | 82  | CB  | LEU | A | 13 | 32.230 | 30.549 | 23.534 | 1.00 | 8.86  | A |
| ATOM | 83  | CG  | LEU | A | 13 | 31.082 | 29.888 | 22.769 | 1.00 | 8.97  | A |
| ATOM | 84  | CD1 | LEU | A | 13 | 31.649 | 28.807 | 21.805 | 1.00 | 12.12 | A |
| ATOM | 85  | CD2 | LEU | A | 13 | 30.101 | 29.268 | 23.753 | 1.00 | 12.69 | A |
| ATOM | 86  | C   | LEU | A | 13 | 32.371 | 32.292 | 21.750 | 1.00 | 9.01  | A |
| ATOM | 87  | O   | LEU | A | 13 | 32.293 | 32.064 | 20.536 | 1.00 | 10.60 | A |
| ATOM | 88  | N   | TYR | A | 14 | 31.761 | 33.329 | 22.305 | 1.00 | 10.47 | A |
| ATOM | 89  | CA  | TYR | A | 14 | 30.920 | 34.195 | 21.482 | 1.00 | 9.03  | A |
| ATOM | 90  | CB  | TYR | A | 14 | 30.029 | 35.087 | 22.352 | 1.00 | 8.38  | A |
| ATOM | 91  | CG  | TYR | A | 14 | 29.091 | 34.293 | 23.253 | 1.00 | 11.48 | A |
| ATOM | 92  | CD1 | TYR | A | 14 | 28.499 | 33.109 | 22.806 | 1.00 | 12.01 | A |
| ATOM | 93  | CE1 | TYR | A | 14 | 27.671 | 32.341 | 23.642 | 1.00 | 10.45 | A |
| ATOM | 94  | CD2 | TYR | A | 14 | 28.824 | 34.706 | 24.564 | 1.00 | 10.30 | A |
| ATOM | 95  | CE2 | TYR | A | 14 | 27.998 | 33.948 | 25.403 | 1.00 | 10.35 | A |
| ATOM | 96  | CZ  | TYR | A | 14 | 27.430 | 32.766 | 24.933 | 1.00 | 8.21  | A |
| ATOM | 97  | OH  | TYR | A | 14 | 26.628 | 32.014 | 25.757 | 1.00 | 8.65  | A |
| ATOM | 98  | C   | TYR | A | 14 | 31.715 | 35.036 | 20.489 | 1.00 | 9.67  | A |
| ATOM | 99  | O   | TYR | A | 14 | 31.142 | 35.538 | 19.515 | 1.00 | 8.36  | A |
| ATOM | 100 | N   | LEU | A | 15 | 33.021 | 35.184 | 20.738 | 1.00 | 8.53  | A |
| ATOM | 101 | CA  | LEU | A | 15 | 33.904 | 35.936 | 19.838 | 1.00 | 9.45  | A |
| ATOM | 102 | CB  | LEU | A | 15 | 35.087 | 36.564 | 20.601 | 1.00 | 8.09  | A |
| ATOM | 103 | CG  | LEU | A | 15 | 34.742 | 37.802 | 21.433 | 1.00 | 14.85 | A |
| ATOM | 104 | CD1 | LEU | A | 15 | 35.932 | 38.141 | 22.306 | 1.00 | 16.07 | A |
| ATOM | 105 | CD2 | LEU | A | 15 | 34.364 | 38.990 | 20.510 | 1.00 | 12.61 | A |
| ATOM | 106 | C   | LEU | A | 15 | 34.467 | 35.018 | 18.756 | 1.00 | 16.00 | A |
| ATOM | 107 | O   | LEU | A | 15 | 35.174 | 35.466 | 17.859 | 1.00 | 16.13 | A |
| ATOM | 108 | N   | THR | A | 16 | 34.178 | 33.729 | 18.848 | 1.00 | 11.70 | A |
| ATOM | 109 | CA  | THR | A | 16 | 34.681 | 32.791 | 17.853 | 1.00 | 11.09 | A |
| ATOM | 110 | CB  | THR | A | 16 | 34.523 | 31.334 | 18.371 | 1.00 | 11.33 | A |
| ATOM | 111 | OG1 | THR | A | 16 | 35.406 | 31.142 | 19.484 | 1.00 | 13.08 | A |
| ATOM | 112 | CG2 | THR | A | 16 | 34.848 | 30.314 | 17.291 | 1.00 | 11.23 | A |
| ATOM | 113 | C   | THR | A | 16 | 33.906 | 32.997 | 16.549 | 1.00 | 12.10 | A |
| ATOM | 114 | O   | THR | A | 16 | 32.671 | 32.996 | 16.540 | 1.00 | 12.20 | A |
| ATOM | 115 | N   | PRO | A | 17 | 34.620 | 33.158 | 15.420 | 1.00 | 14.18 | A |
| ATOM | 116 | CD  | PRO | A | 17 | 36.085 | 33.162 | 15.251 | 1.00 | 14.83 | A |
| ATOM | 117 | CA  | PRO | A | 17 | 33.933 | 33.367 | 14.137 | 1.00 | 17.90 | A |
| ATOM | 118 | CB  | PRO | A | 17 | 35.068 | 33.292 | 13.113 | 1.00 | 20.97 | A |
| ATOM | 119 | CG  | PRO | A | 17 | 36.251 | 33.842 | 13.890 | 1.00 | 21.64 | A |
| ATOM | 120 | C   | PRO | A | 17 | 32.830 | 32.341 | 13.854 | 1.00 | 14.42 | A |
| ATOM | 121 | O   | PRO | A | 17 | 33.027 | 31.143 | 14.066 | 1.00 | 14.18 | A |
| ATOM | 122 | N   | ASP | A | 18 | 31.673 | 32.836 | 13.414 | 1.00 | 15.17 | A |
| ATOM | 123 | CA  | ASP | A | 18 | 30.515 | 32.020 | 13.058 | 1.00 | 19.19 | A |
| ATOM | 124 | CB  | ASP | A | 18 | 30.932 | 30.829 | 12.169 | 1.00 | 23.04 | A |
| ATOM | 125 | CG  | ASP | A | 18 | 31.649 | 31.260 | 10.885 | 1.00 | 30.30 | A |
| ATOM | 126 | OD1 | ASP | A | 18 | 31.214 | 32.238 | 10.239 | 1.00 | 30.86 | A |
| ATOM | 127 | OD2 | ASP | A | 18 | 32.645 | 30.599 | 10.511 | 1.00 | 39.65 | A |
| ATOM | 128 | C   | ASP | A | 18 | 29.657 | 31.479 | 14.212 | 1.00 | 13.08 | A |
| ATOM | 129 | O   | ASP | A | 18 | 28.651 | 30.833 | 13.958 | 1.00 | 13.28 | A |
| ATOM | 130 | N   | VAL | A | 19 | 30.041 | 31.709 | 15.466 | 1.00 | 13.07 | A |
| ATOM | 131 | CA  | VAL | A | 19 | 29.199 | 31.221 | 16.570 | 1.00 | 8.94  | A |
| ATOM | 132 | CB  | VAL | A | 19 | 29.976 | 31.225 | 17.911 | 1.00 | 9.65  | A |
| ATOM | 133 | CG1 | VAL | A | 19 | 29.014 | 31.123 | 19.098 | 1.00 | 11.73 | A |
| ATOM | 134 | CG2 | VAL | A | 19 | 30.930 | 30.026 | 17.923 | 1.00 | 11.99 | A |
| ATOM | 135 | C   | VAL | A | 19 | 27.971 | 32.126 | 16.613 | 1.00 | 11.81 | A |
| ATOM | 136 | O   | VAL | A | 19 | 26.829 | 31.655 | 16.707 | 1.00 | 11.21 | A |
| ATOM | 137 | N   | LEU | A | 20 | 28.198 | 33.434 | 16.567 | 1.00 | 10.93 | A |
| ATOM | 138 | CA  | LEU | A | 20 | 27.077 | 34.363 | 16.486 | 1.00 | 8.58  | A |
| ATOM | 139 | CB  | LEU | A | 20 | 27.439 | 35.730 | 17.084 | 1.00 | 13.44 | A |
| ATOM | 140 | CG  | LEU | A | 20 | 27.677 | 35.767 | 18.601 | 1.00 | 14.24 | A |
| ATOM | 141 | CD1 | LEU | A | 20 | 27.863 | 37.222 | 19.084 | 1.00 | 13.26 | A |
| ATOM | 142 | CD2 | LEU | A | 20 | 26.480 | 35.130 | 19.315 | 1.00 | 11.94 | A |
| ATOM | 143 | C   | LEU | A | 20 | 26.857 | 34.470 | 14.969 | 1.00 | 15.21 | A |
| ATOM | 144 | O   | LEU | A | 20 | 27.836 | 34.550 | 14.196 | 1.00 | 11.72 | A |
| ATOM | 145 | N   | THR | A | 21 | 25.596 | 34.455 | 14.540 | 1.00 | 14.05 | A |
| ATOM | 146 | CA  | THR | A | 21 | 25.268 | 34.511 | 13.114 | 1.00 | 12.27 | A |
| ATOM | 147 | CB  | THR | A | 21 | 24.006 | 33.653 | 12.865 | 1.00 | 16.46 | A |
| ATOM | 148 | OG1 | THR | A | 21 | 22.966 | 34.044 | 13.774 | 1.00 | 13.53 | A |
| ATOM | 149 | CG2 | THR | A | 21 | 24.326 | 32.173 | 13.121 | 1.00 | 17.80 | A |
| ATOM | 150 | C   | THR | A | 21 | 25.121 | 35.937 | 12.509 | 1.00 | 14.67 | A |
| ATOM | 151 | O   | THR | A | 21 | 25.452 | 36.928 | 13.148 | 1.00 | 12.04 | A |

FIGURE 5 (suite)

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 152 | N   | ALA | A | 22 | 24.663 | 36.037 | 11.265 | 1.00 | 12.98 | A |
| ATOM | 153 | CA  | ALA | A | 22 | 24.523 | 37.335 | 10.594 | 1.00 | 12.25 | A |
| ATOM | 154 | CB  | ALA | A | 22 | 23.913 | 37.146 | 9.208  | 1.00 | 15.06 | A |
| ATOM | 155 | C   | ALA | A | 22 | 23.749 | 38.418 | 11.337 | 1.00 | 10.99 | A |
| ATOM | 156 | O   | ALA | A | 22 | 22.688 | 38.174 | 11.916 | 1.00 | 15.12 | A |
| ATOM | 157 | N   | GLY | A | 23 | 24.285 | 39.636 | 11.292 | 1.00 | 13.67 | A |
| ATOM | 158 | CA  | GLY | A | 23 | 23.631 | 40.753 | 11.951 | 1.00 | 14.86 | A |
| ATOM | 159 | C   | GLY | A | 23 | 24.068 | 41.057 | 13.371 | 1.00 | 14.29 | A |
| ATOM | 160 | O   | GLY | A | 23 | 23.775 | 42.138 | 13.894 | 1.00 | 15.41 | A |
| ATOM | 161 | N   | PHE | A | 24 | 24.760 | 40.116 | 14.001 | 1.00 | 12.44 | A |
| ATOM | 162 | CA  | PHE | A | 24 | 25.238 | 40.283 | 15.363 | 1.00 | 14.48 | A |
| ATOM | 163 | CB  | PHE | A | 24 | 25.424 | 38.899 | 16.020 | 1.00 | 9.89  | A |
| ATOM | 164 | CG  | PHE | A | 24 | 24.156 | 38.276 | 16.527 | 1.00 | 12.35 | A |
| ATOM | 165 | CD1 | PHE | A | 24 | 23.225 | 37.734 | 15.644 | 1.00 | 6.46  | A |
| ATOM | 166 | CD2 | PHE | A | 24 | 23.888 | 38.237 | 17.898 | 1.00 | 12.73 | A |
| ATOM | 157 | CE1 | PHE | A | 24 | 22.035 | 37.153 | 16.125 | 1.00 | 11.12 | A |
| ATOM | 168 | CE2 | PHE | A | 24 | 22.695 | 37.662 | 18.397 | 1.00 | 7.42  | A |
| ATOM | 169 | CZ  | PHE | A | 24 | 21.772 | 37.118 | 17.502 | 1.00 | 11.79 | A |
| ATOM | 170 | C   | PHE | A | 24 | 26.584 | 41.030 | 15.444 | 1.00 | 14.36 | A |
| ATOM | 171 | O   | PHE | A | 24 | 27.569 | 40.592 | 14.850 | 1.00 | 12.41 | A |
| ATOM | 172 | N   | ALA | A | 25 | 26.630 | 42.141 | 16.183 | 1.00 | 14.60 | A |
| ATOM | 173 | CA  | ALA | A | 25 | 27.881 | 42.875 | 16.378 | 1.00 | 13.54 | A |
| ATOM | 174 | CB  | ALA | A | 25 | 27.606 | 44.233 | 17.024 | 1.00 | 15.19 | A |
| ATOM | 175 | C   | ALA | A | 25 | 28.752 | 42.031 | 17.315 | 1.00 | 12.48 | A |
| ATOM | 176 | O   | ALA | A | 25 | 28.240 | 41.155 | 18.023 | 1.00 | 12.61 | A |
| ATOM | 177 | N   | PRO | A | 26 | 30.067 | 42.289 | 17.348 | 1.00 | 11.27 | A |
| ATOM | 178 | CD  | PRO | A | 26 | 30.837 | 43.202 | 16.476 | 1.00 | 13.96 | A |
| ATOM | 179 | CA  | PRO | A | 26 | 30.952 | 41.507 | 18.231 | 1.00 | 12.70 | A |
| ATOM | 180 | CB  | PRO | A | 26 | 32.334 | 42.117 | 17.989 | 1.00 | 14.99 | A |
| ATOM | 181 | CG  | PRO | A | 26 | 32.241 | 42.582 | 16.519 | 1.00 | 19.22 | A |
| ATOM | 182 | C   | PRO | A | 26 | 30.536 | 41.602 | 19.699 | 1.00 | 10.57 | A |
| ATOM | 183 | O   | PRO | A | 26 | 30.222 | 42.681 | 20.192 | 1.00 | 10.54 | A |
| ATOM | 184 | N   | TYR | A | 27 | 30.529 | 40.456 | 20.367 | 1.00 | 8.04  | A |
| ATOM | 185 | CA  | TYR | A | 27 | 30.161 | 40.345 | 21.793 | 1.00 | 9.13  | A |
| ATOM | 186 | CB  | TYR | A | 27 | 30.294 | 38.886 | 22.231 | 1.00 | 8.74  | A |
| ATOM | 187 | CG  | TYR | A | 27 | 29.824 | 38.612 | 23.648 | 1.00 | 5.12  | A |
| ATOM | 188 | CD1 | TYR | A | 27 | 28.469 | 38.512 | 23.938 | 1.00 | 6.81  | A |
| ATOM | 189 | CE1 | TYR | A | 27 | 28.024 | 38.224 | 25.247 | 1.00 | 9.00  | A |
| ATOM | 190 | CD2 | TYR | A | 27 | 30.741 | 38.423 | 24.682 | 1.00 | 5.70  | A |
| ATOM | 191 | CE2 | TYR | A | 27 | 30.310 | 38.131 | 25.992 | 1.00 | 7.78  | A |
| ATOM | 192 | CZ  | TYR | A | 27 | 28.948 | 38.032 | 26.259 | 1.00 | 9.36  | A |
| ATOM | 193 | OH  | TYR | A | 27 | 28.502 | 37.709 | 27.532 | 1.00 | 8.37  | A |
| ATOM | 194 | C   | TYR | A | 27 | 31.081 | 41.207 | 22.675 | 1.00 | 10.49 | A |
| ATOM | 195 | O   | TYR | A | 27 | 32.297 | 41.207 | 22.494 | 1.00 | 9.91  | A |
| ATOM | 196 | N   | ILE | A | 28 | 30.510 | 41.931 | 23.635 | 1.00 | 8.97  | A |
| ATOM | 197 | CA  | ILE | A | 28 | 31.324 | 42.765 | 24.517 | 1.00 | 12.31 | A |
| ATOM | 198 | CB  | ILE | A | 28 | 30.801 | 44.225 | 24.521 | 1.00 | 13.61 | A |
| ATOM | 199 | CG2 | ILE | A | 28 | 31.657 | 45.098 | 25.459 | 1.00 | 13.95 | A |
| ATOM | 200 | CG1 | ILE | A | 28 | 30.871 | 44.793 | 23.095 | 1.00 | 11.91 | A |
| ATOM | 201 | CD1 | ILE | A | 28 | 30.192 | 46.146 | 22.915 | 1.00 | 12.92 | A |
| ATOM | 202 | C   | ILE | A | 28 | 31.333 | 42.191 | 25.942 | 1.00 | 13.14 | A |
| ATOM | 203 | O   | ILE | A | 28 | 30.315 | 42.189 | 26.622 | 1.00 | 8.79  | A |
| ATOM | 204 | N   | GLY | A | 29 | 32.499 | 41.706 | 26.373 | 1.00 | 13.23 | A |
| ATOM | 205 | CA  | GLY | A | 29 | 32.630 | 41.105 | 27.695 | 1.00 | 15.83 | A |
| ATOM | 206 | C   | GLY | A | 29 | 32.868 | 42.127 | 28.791 | 1.00 | 16.10 | A |
| ATOM | 207 | O   | GLY | A | 29 | 33.915 | 42.794 | 28.826 | 1.00 | 12.27 | A |
| ATOM | 208 | N   | THR | A | 30 | 31.900 | 42.234 | 29.697 | 1.00 | 8.70  | A |
| ATOM | 209 | CA  | THR | A | 30 | 31.966 | 43.200 | 30.783 | 1.00 | 10.71 | A |
| ATOM | 210 | CB  | THR | A | 30 | 31.061 | 44.442 | 30.473 | 1.00 | 11.83 | A |
| ATOM | 211 | OG1 | THR | A | 30 | 29.703 | 44.014 | 30.222 | 1.00 | 16.91 | A |
| ATOM | 212 | CG2 | THR | A | 30 | 31.607 | 45.235 | 29.249 | 1.00 | 8.83  | A |
| ATOM | 213 | C   | THR | A | 30 | 31.538 | 42.640 | 32.147 | 1.00 | 11.78 | A |
| ATOM | 214 | O   | THR | A | 30 | 31.532 | 43.378 | 33.135 | 1.00 | 11.34 | A |
| ATOM | 215 | N   | GLY | A | 31 | 31.187 | 41.352 | 32.210 | 1.00 | 10.41 | A |
| ATOM | 216 | CA  | GLY | A | 31 | 30.729 | 40.789 | 33.473 | 1.00 | 8.40  | A |
| ATOM | 217 | C   | GLY | A | 31 | 29.208 | 40.604 | 33.467 | 1.00 | 9.64  | A |
| ATOM | 218 | O   | GLY | A | 31 | 28.478 | 41.396 | 32.862 | 1.00 | 8.01  | A |
| ATOM | 219 | N   | SER | A | 32 | 28.718 | 39.566 | 34.138 | 1.00 | 7.93  | A |
| ATOM | 220 | CA  | SER | A | 32 | 27.274 | 39.297 | 34.143 | 1.00 | 4.39  | A |
| ATOM | 221 | CB  | SER | A | 32 | 26.961 | 37.954 | 34.832 | 1.00 | 2.86  | A |
| ATOM | 222 | OG  | SER | A | 32 | 27.538 | 36.876 | 34.125 | 1.00 | 6.73  | A |
| ATOM | 223 | C   | SER | A | 32 | 26.440 | 40.386 | 34.793 | 1.00 | 7.61  | A |
| ATOM | 224 | O   | SER | A | 32 | 25.321 | 40.626 | 34.354 | 1.00 | 9.70  | A |
| ATOM | 225 | N   | GLY | A | 33 | 26.984 | 41.052 | 35.811 | 1.00 | 8.20  | A |
| ATOM | 226 | CA  | GLY | A | 33 | 26.256 | 42.121 | 36.506 | 1.00 | 6.91  | A |

FIGURE 5 (suite)

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 227 | C   | GLY | A | 33 | 25.942 | 43.235 | 35.524 | 1.00 | 9.16  | A |
| ATOM | 228 | O   | GLY | A | 33 | 24.799 | 43.708 | 35.429 | 1.00 | 9.95  | A |
| ATOM | 229 | N   | LYS | A | 34 | 26.943 | 43.633 | 34.749 | 1.00 | 10.60 | A |
| ATOM | 230 | CA  | LYS | A | 34 | 26.710 | 44.681 | 33.758 | 1.00 | 8.52  | A |
| ATOM | 231 | CB  | LYS | A | 34 | 28.040 | 45.240 | 33.250 | 1.00 | 7.07  | A |
| ATOM | 232 | CG  | LYS | A | 34 | 28.667 | 46.220 | 34.250 | 1.00 | 12.80 | A |
| ATOM | 233 | CD  | LYS | A | 34 | 29.957 | 46.854 | 33.703 | 1.00 | 10.66 | A |
| ATOM | 234 | CE  | LYS | A | 34 | 30.597 | 47.768 | 34.748 | 1.00 | 10.90 | A |
| ATOM | 235 | NZ  | LYS | A | 34 | 29.700 | 48.890 | 35.066 | 1.00 | 23.47 | A |
| ATOM | 236 | C   | LYS | A | 34 | 25.848 | 44.201 | 32.601 | 1.00 | 12.94 | A |
| ATOM | 237 | O   | LYS | A | 34 | 25.070 | 44.977 | 32.043 | 1.00 | 9.59  | A |
| ATOM | 238 | N   | GLY | A | 35 | 25.983 | 42.928 | 32.236 | 1.00 | 9.69  | A |
| ATOM | 239 | CA  | GLY | A | 35 | 25.158 | 42.386 | 31.162 | 1.00 | 7.50  | A |
| ATOM | 240 | C   | GLY | A | 35 | 23.677 | 42.414 | 31.542 | 1.00 | 9.68  | A |
| ATOM | 241 | O   | GLY | A | 35 | 22.831 | 42.767 | 30.717 | 1.00 | 9.00  | A |
| ATOM | 242 | N   | LYS | A | 36 | 23.340 | 42.077 | 32.787 | 1.00 | 8.56  | A |
| ATOM | 243 | CA  | LYS | A | 36 | 21.929 | 42.089 | 33.173 | 1.00 | 7.26  | A |
| ATOM | 244 | CB  | LYS | A | 36 | 21.709 | 41.393 | 34.533 | 1.00 | 9.15  | A |
| ATOM | 245 | CG  | LYS | A | 36 | 21.954 | 39.861 | 34.445 | 1.00 | 5.28  | A |
| ATOM | 246 | CD  | LYS | A | 36 | 21.394 | 39.069 | 35.662 | 1.00 | 6.85  | A |
| ATOM | 247 | CE  | LYS | A | 36 | 21.990 | 39.576 | 36.986 | 1.00 | 11.53 | A |
| ATOM | 248 | NZ  | LYS | A | 36 | 21.397 | 38.945 | 38.221 | 1.00 | 11.99 | A |
| ATOM | 249 | C   | LYS | A | 36 | 21.409 | 43.527 | 33.204 | 1.00 | 11.18 | A |
| ATOM | 250 | O   | LYS | A | 36 | 20.311 | 43.787 | 32.724 | 1.00 | 14.03 | A |
| ATOM | 251 | N   | ILE | A | 37 | 22.190 | 44.459 | 33.749 | 1.00 | 9.12  | A |
| ATOM | 252 | CA  | ILE | A | 37 | 21.752 | 45.854 | 33.766 | 1.00 | 11.15 | A |
| ATOM | 253 | CB  | ILE | A | 37 | 22.778 | 46.779 | 34.462 | 1.00 | 10.46 | A |
| ATOM | 254 | CG2 | ILE | A | 37 | 22.424 | 48.252 | 34.197 | 1.00 | 11.32 | A |
| ATOM | 255 | CG1 | ILE | A | 37 | 22.774 | 46.522 | 35.972 | 1.00 | 9.50  | A |
| ATOM | 256 | CD1 | ILE | A | 37 | 24.024 | 47.029 | 36.669 | 1.00 | 15.62 | A |
| ATOM | 257 | C   | ILE | A | 37 | 21.563 | 46.368 | 32.325 | 1.00 | 11.78 | A |
| ATOM | 258 | O   | ILE | A | 37 | 20.570 | 47.017 | 32.018 | 1.00 | 11.36 | A |
| ATOM | 259 | N   | ALA | A | 38 | 22.518 | 46.071 | 31.452 | 1.00 | 9.31  | A |
| ATOM | 260 | CA  | ALA | A | 38 | 22.438 | 46.539 | 30.063 | 1.00 | 10.19 | A |
| ATOM | 261 | CB  | ALA | A | 38 | 23.650 | 46.016 | 29.269 | 1.00 | 10.93 | A |
| ATOM | 262 | C   | ALA | A | 38 | 21.129 | 46.102 | 29.375 | 1.00 | 9.69  | A |
| ATOM | 263 | O   | ALA | A | 38 | 20.447 | 46.899 | 28.712 | 1.00 | 8.41  | A |
| ATOM | 264 | N   | PHE | A | 39 | 20.771 | 44.831 | 29.541 | 1.00 | 8.70  | A |
| ATOM | 265 | CA  | PHE | A | 39 | 19.566 | 44.327 | 28.914 | 1.00 | 9.40  | A |
| ATOM | 266 | CB  | PHE | A | 39 | 19.549 | 42.787 | 28.888 | 1.00 | 9.06  | A |
| ATOM | 267 | CG  | PHE | A | 39 | 18.287 | 42.214 | 28.270 | 1.00 | 7.16  | A |
| ATOM | 268 | CD1 | PHE | A | 39 | 18.223 | 41.953 | 26.896 | 1.00 | 8.56  | A |
| ATOM | 269 | CD2 | PHE | A | 39 | 17.146 | 42.000 | 29.051 | 1.00 | 8.19  | A |
| ATOM | 270 | CE1 | PHE | A | 39 | 17.035 | 41.481 | 26.306 | 1.00 | 9.12  | A |
| ATOM | 271 | CE2 | PHE | A | 39 | 15.947 | 41.530 | 28.479 | 1.00 | 9.01  | A |
| ATOM | 272 | CZ  | PHE | A | 39 | 15.888 | 41.269 | 27.101 | 1.00 | 8.28  | A |
| ATOM | 273 | C   | PHE | A | 39 | 18.304 | 44.790 | 29.508 | 1.00 | 12.15 | A |
| ATOM | 274 | O   | PHE | A | 39 | 17.398 | 45.313 | 28.972 | 1.00 | 10.76 | A |
| ATOM | 275 | N   | LEU | A | 40 | 18.246 | 44.602 | 30.920 | 1.00 | 8.71  | A |
| ATOM | 276 | CA  | LEU | A | 40 | 17.034 | 44.938 | 31.678 | 1.00 | 8.94  | A |
| ATOM | 277 | CB  | LEU | A | 40 | 17.204 | 44.513 | 33.144 | 1.00 | 7.80  | A |
| ATOM | 278 | CG  | LEU | A | 40 | 17.342 | 43.005 | 33.400 | 1.00 | 10.06 | A |
| ATOM | 279 | CD1 | LEU | A | 40 | 17.809 | 42.781 | 34.887 | 1.00 | 6.45  | A |
| ATOM | 280 | CD2 | LEU | A | 40 | 16.006 | 42.296 | 33.132 | 1.00 | 12.55 | A |
| ATOM | 281 | C   | LEU | A | 40 | 16.526 | 46.403 | 31.632 | 1.00 | 10.63 | A |
| ATOM | 282 | O   | LEU | A | 40 | 15.430 | 46.730 | 31.629 | 1.00 | 11.89 | A |
| ATOM | 283 | N   | GLU | A | 41 | 17.604 | 47.291 | 31.586 | 1.00 | 10.88 | A |
| ATOM | 284 | CA  | GLU | A | 41 | 17.294 | 48.717 | 31.551 | 1.00 | 9.10  | A |
| ATOM | 285 | CB  | GLU | A | 41 | 18.053 | 49.436 | 32.669 | 1.00 | 13.20 | A |
| ATOM | 286 | CG  | GLU | A | 41 | 17.802 | 48.829 | 34.036 | 1.00 | 11.00 | A |
| ATOM | 287 | CD  | GLU | A | 41 | 18.671 | 49.429 | 35.131 | 1.00 | 22.54 | A |
| ATOM | 288 | OE1 | GLU | A | 41 | 18.975 | 48.713 | 36.103 | 1.00 | 27.36 | A |
| ATOM | 289 | OE2 | GLU | A | 41 | 19.037 | 50.616 | 35.043 | 1.00 | 22.49 | A |
| ATOM | 290 | C   | GLU | A | 41 | 17.633 | 49.361 | 30.218 | 1.00 | 12.72 | A |
| ATOM | 291 | O   | GLU | A | 41 | 17.505 | 50.576 | 30.066 | 1.00 | 13.60 | A |
| ATOM | 292 | N   | ASN | A | 42 | 18.010 | 48.537 | 29.238 | 1.00 | 11.74 | A |
| ATOM | 293 | CA  | ASN | A | 42 | 18.463 | 49.008 | 27.923 | 1.00 | 11.79 | A |
| ATOM | 294 | CB  | ASN | A | 42 | 17.322 | 49.494 | 27.022 | 1.00 | 14.08 | A |
| ATOM | 295 | CG  | ASN | A | 42 | 17.824 | 49.897 | 25.642 | 1.00 | 16.54 | A |
| ATOM | 296 | OD1 | ASN | A | 42 | 18.885 | 49.428 | 25.189 | 1.00 | 15.67 | A |
| ATOM | 297 | ND2 | ASN | A | 42 | 17.076 | 50.763 | 24.960 | 1.00 | 14.22 | A |
| ATOM | 298 | C   | ASN | A | 42 | 19.486 | 50.126 | 28.091 | 1.00 | 16.68 | A |
| ATOM | 299 | O   | ASN | A | 42 | 19.300 | 51.260 | 27.631 | 1.00 | 14.27 | A |
| ATOM | 300 | N   | SER | A | 43 | 20.578 | 49.789 | 28.767 | 1.00 | 14.51 | A |

FIGURE 5 (suite)

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 301 | CA  | SER | A | 43 | 21.665 | 50.740 | 29.001 | 1.00 | 14.54 | A |
| ATOM | 302 | CB  | SER | A | 43 | 21.920 | 50.874 | 30.520 | 1.00 | 19.90 | A |
| ATOM | 303 | OG  | SER | A | 43 | 20.922 | 51.662 | 31.162 | 1.00 | 26.26 | A |
| ATOM | 304 | C   | SER | A | 43 | 22.965 | 50.327 | 28.302 | 1.00 | 13.78 | A |
| ATOM | 305 | O   | SER | A | 43 | 23.790 | 49.633 | 28.891 | 1.00 | 10.60 | A |
| ATOM | 306 | N   | TYR | A | 44 | 23.168 | 50.755 | 27.056 | 1.00 | 9.73  | A |
| ATOM | 307 | CA  | TYR | A | 44 | 24.396 | 50.401 | 26.361 | 1.00 | 10.86 | A |
| ATOM | 308 | CB  | TYR | A | 44 | 24.330 | 50.880 | 24.904 | 1.00 | 10.54 | A |
| ATOM | 309 | CG  | TYR | A | 44 | 25.414 | 50.311 | 24.034 | 1.00 | 12.22 | A |
| ATOM | 310 | CD1 | TYR | A | 44 | 26.631 | 50.983 | 23.857 | 1.00 | 12.57 | A |
| ATOM | 311 | CE1 | TYR | A | 44 | 27.625 | 50.469 | 23.011 | 1.00 | 10.91 | A |
| ATOM | 312 | CD2 | TYR | A | 44 | 25.217 | 49.106 | 23.357 | 1.00 | 10.34 | A |
| ATOM | 313 | CE2 | TYR | A | 44 | 26.201 | 48.587 | 22.517 | 1.00 | 11.21 | A |
| ATOM | 314 | CZ  | TYR | A | 44 | 27.394 | 49.267 | 22.347 | 1.00 | 14.12 | A |
| ATOM | 315 | OH  | TYR | A | 44 | 28.357 | 48.725 | 21.524 | 1.00 | 11.54 | A |
| ATOM | 316 | C   | TYR | A | 44 | 25.650 | 50.971 | 27.026 | 1.00 | 8.02  | A |
| ATOM | 317 | O   | TYR | A | 44 | 26.775 | 50.515 | 26.756 | 1.00 | 10.36 | A |
| ATOM | 318 | N   | ASN | A | 45 | 25.484 | 51.941 | 27.917 | 1.00 | 8.55  | A |
| ATOM | 319 | CA  | ASN | A | 45 | 26.657 | 52.547 | 28.535 | 1.00 | 14.36 | A |
| ATOM | 320 | CB  | ASN | A | 45 | 26.271 | 53.811 | 29.337 | 1.00 | 8.69  | A |
| ATOM | 321 | CG  | ASN | A | 45 | 25.707 | 53.503 | 30.708 | 1.00 | 11.69 | A |
| ATOM | 322 | OD1 | ASN | A | 45 | 25.048 | 52.488 | 30.910 | 1.00 | 13.56 | A |
| ATOM | 323 | ND2 | ASN | A | 45 | 25.934 | 54.411 | 31.655 | 1.00 | 14.48 | A |
| ATOM | 324 | C   | ASN | A | 45 | 27.423 | 51.535 | 29.388 | 1.00 | 13.91 | A |
| ATOM | 325 | O   | ASN | A | 45 | 28.573 | 51.781 | 29.755 | 1.00 | 11.13 | A |
| ATOM | 326 | N   | GLN | A | 46 | 26.788 | 50.393 | 29.681 | 1.00 | 8.83  | A |
| ATOM | 327 | CA  | GLN | A | 46 | 27.462 | 49.337 | 30.435 | 1.00 | 11.62 | A |
| ATOM | 328 | CB  | GLN | A | 46 | 26.421 | 48.390 | 31.080 | 1.00 | 10.13 | A |
| ATOM | 329 | CG  | GLN | A | 46 | 25.487 | 49.076 | 32.083 | 1.00 | 14.66 | A |
| ATOM | 330 | CD  | GLN | A | 46 | 26.259 | 49.792 | 33.170 | 1.00 | 18.72 | A |
| ATOM | 331 | OE1 | GLN | A | 46 | 26.983 | 49.165 | 33.937 | 1.00 | 18.65 | A |
| ATOM | 332 | NE2 | GLN | A | 46 | 26.133 | 51.116 | 33.228 | 1.00 | 16.99 | A |
| ATOM | 333 | C   | GLN | A | 46 | 28.408 | 48.543 | 29.491 | 1.00 | 10.06 | A |
| ATOM | 334 | O   | GLN | A | 46 | 29.275 | 47.818 | 29.956 | 1.00 | 10.43 | A |
| ATOM | 335 | N   | PHE | A | 47 | 28.232 | 48.691 | 28.174 | 1.00 | 8.72  | A |
| ATOM | 336 | CA  | PHE | A | 47 | 29.055 | 48.025 | 27.148 | 1.00 | 7.46  | A |
| ATOM | 337 | CB  | PHE | A | 47 | 28.191 | 47.487 | 25.992 | 1.00 | 7.56  | A |
| ATOM | 338 | CG  | PHE | A | 47 | 27.271 | 46.349 | 26.366 | 1.00 | 12.11 | A |
| ATOM | 339 | CD1 | PHE | A | 47 | 27.433 | 45.651 | 27.559 | 1.00 | 11.35 | A |
| ATOM | 340 | CD2 | PHE | A | 47 | 26.268 | 45.945 | 25.474 | 1.00 | 14.21 | A |
| ATOM | 341 | CE1 | PHE | A | 47 | 26.616 | 44.567 | 27.861 | 1.00 | 9.31  | A |
| ATOM | 342 | CE2 | PHE | A | 47 | 25.442 | 44.859 | 25.761 | 1.00 | 9.84  | A |
| ATOM | 343 | CZ  | PHE | A | 47 | 25.617 | 44.167 | 26.959 | 1.00 | 10.19 | A |
| ATOM | 344 | C   | PHE | A | 47 | 30.053 | 48.988 | 26.484 | 1.00 | 12.94 | A |
| ATOM | 345 | O   | PHE | A | 47 | 31.109 | 48.580 | 26.022 | 1.00 | 14.11 | A |
| ATOM | 346 | N   | GLY | A | 48 | 29.677 | 50.257 | 26.378 | 1.00 | 11.49 | A |
| ATOM | 347 | CA  | GLY | A | 48 | 30.551 | 51.222 | 25.731 | 1.00 | 13.51 | A |
| ATOM | 348 | C   | GLY | A | 48 | 30.027 | 52.642 | 25.833 | 1.00 | 15.44 | A |
| ATOM | 349 | O   | GLY | A | 48 | 28.999 | 52.908 | 26.459 | 1.00 | 16.60 | A |
| ATOM | 350 | N   | THR | A | 49 | 30.722 | 53.566 | 25.187 | 1.00 | 14.37 | A |
| ATOM | 351 | CA  | THR | A | 49 | 30.333 | 54.967 | 25.256 | 1.00 | 13.58 | A |
| ATOM | 352 | CB  | THR | A | 49 | 31.576 | 55.843 | 25.161 | 1.00 | 14.46 | A |
| ATOM | 353 | OG1 | THR | A | 49 | 32.234 | 55.567 | 23.924 | 1.00 | 15.00 | A |
| ATOM | 354 | CG2 | THR | A | 49 | 32.558 | 55.524 | 26.322 | 1.00 | 13.17 | A |
| ATOM | 355 | C   | THR | A | 49 | 29.301 | 55.436 | 24.216 | 1.00 | 14.30 | A |
| ATOM | 356 | O   | THR | A | 49 | 28.716 | 56.511 | 24.370 | 1.00 | 12.47 | A |
| ATOM | 357 | N   | ASN | A | 50 | 29.062 | 54.659 | 23.162 | 1.00 | 13.09 | A |
| ATOM | 358 | CA  | ASN | A | 50 | 28.076 | 55.116 | 22.173 | 1.00 | 14.85 | A |
| ATOM | 359 | CB  | ASN | A | 50 | 28.324 | 54.519 | 20.785 | 1.00 | 15.63 | A |
| ATOM | 360 | CG  | ASN | A | 50 | 27.379 | 55.096 | 19.739 | 1.00 | 18.88 | A |
| ATOM | 361 | OD1 | ASN | A | 50 | 26.472 | 55.883 | 20.059 | 1.00 | 19.28 | A |
| ATOM | 362 | ND2 | ASN | A | 50 | 27.574 | 54.707 | 18.489 | 1.00 | 19.28 | A |
| ATOM | 363 | C   | ASN | A | 50 | 26.669 | 54.751 | 22.615 | 1.00 | 14.82 | A |
| ATOM | 364 | O   | ASN | A | 50 | 26.099 | 53.739 | 22.187 | 1.00 | 14.58 | A |
| ATOM | 365 | N   | THR | A | 51 | 26.097 | 55.608 | 23.443 | 1.00 | 13.25 | A |
| ATOM | 366 | CA  | THR | A | 51 | 24.782 | 55.377 | 23.988 | 1.00 | 15.77 | A |
| ATOM | 367 | CB  | THR | A | 51 | 24.595 | 56.210 | 25.242 | 1.00 | 17.96 | A |
| ATOM | 368 | OG1 | THR | A | 51 | 24.937 | 57.574 | 24.973 | 1.00 | 16.18 | A |
| ATOM | 369 | CG2 | THR | A | 51 | 25.506 | 55.684 | 26.332 | 1.00 | 18.64 | A |
| ATOM | 370 | C   | THR | A | 51 | 23.581 | 55.539 | 23.053 | 1.00 | 18.71 | A |
| ATOM | 371 | O   | THR | A | 51 | 22.440 | 55.436 | 23.512 | 1.00 | 19.68 | A |
| ATOM | 372 | N   | THR | A | 52 | 23.820 | 55.795 | 21.761 | 1.00 | 16.82 | A |
| ATOM | 373 | CA  | THR | A | 52 | 22.702 | 55.865 | 20.827 | 1.00 | 19.67 | A |
| ATOM | 374 | CB  | THR | A | 52 | 23.017 | 56.666 | 19.524 | 1.00 | 22.55 | A |
| ATOM | 375 | OG1 | THR | A | 52 | 24.028 | 56.006 | 18.744 | 1.00 | 22.57 | A |

FIGURE 5 (suite)

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 376 | CG2 | THR | A | 52 | 23.460 | 58.081 | 19.875 | 1.00 | 21.07 | A |
| ATOM | 377 | C   | THR | A | 52 | 22.342 | 54.428 | 20.446 | 1.00 | 17.92 | A |
| ATOM | 378 | O   | THR | A | 52 | 21.270 | 54.175 | 19.905 | 1.00 | 17.96 | A |
| ATOM | 379 | N   | LYS | A | 53 | 23.238 | 53.488 | 20.740 | 1.00 | 14.41 | A |
| ATOM | 380 | CA  | LYS | A | 53 | 22.978 | 52.080 | 20.427 | 1.00 | 12.53 | A |
| ATOM | 381 | CB  | LYS | A | 53 | 24.292 | 51.292 | 20.406 | 1.00 | 14.33 | A |
| ATOM | 382 | CG  | LYS | A | 53 | 25.207 | 51.573 | 19.213 | 1.00 | 17.93 | A |
| ATOM | 383 | CD  | LYS | A | 53 | 26.478 | 50.731 | 19.324 | 1.00 | 18.20 | A |
| ATOM | 384 | CE  | LYS | A | 53 | 27.477 | 51.052 | 18.214 | 1.00 | 21.01 | A |
| ATOM | 385 | NZ  | LYS | A | 53 | 26.908 | 50.784 | 16.865 | 1.00 | 22.67 | A |
| ATOM | 386 | C   | LYS | A | 53 | 22.045 | 51.470 | 21.474 | 1.00 | 12.72 | A |
| ATOM | 387 | O   | LYS | A | 53 | 22.075 | 51.869 | 22.635 | 1.00 | 11.93 | A |
| ATOM | 388 | N   | ASP | A | 54 | 21.223 | 50.499 | 21.064 | 1.00 | 13.58 | A |
| ATOM | 389 | CA  | ASP | A | 54 | 20.298 | 49.826 | 21.982 | 1.00 | 10.96 | A |
| ATOM | 390 | CB  | ASP | A | 54 | 18.887 | 49.745 | 21.380 | 1.00 | 12.81 | A |
| ATOM | 391 | CG  | ASP | A | 54 | 18.249 | 51.107 | 21.218 | 1.00 | 19.07 | A |
| ATOM | 392 | OD1 | ASP | A | 54 | 18.010 | 51.529 | 20.059 | 1.00 | 17.31 | A |
| ATOM | 393 | OD2 | ASP | A | 54 | 17.997 | 51.759 | 22.260 | 1.00 | 15.46 | A |
| ATOM | 394 | C   | ASP | A | 54 | 20.819 | 48.416 | 22.246 | 1.00 | 8.44  | A |
| ATOM | 395 | O   | ASP | A | 54 | 21.505 | 47.637 | 21.407 | 1.00 | 14.56 | A |
| ATOM | 396 | N   | VAL | A | 55 | 20.485 | 47.875 | 23.411 | 1.00 | 12.75 | A |
| ATOM | 397 | CA  | VAL | A | 55 | 20.919 | 46.541 | 23.799 | 1.00 | 12.22 | A |
| ATOM | 398 | CB  | VAL | A | 55 | 21.150 | 46.486 | 25.328 | 1.00 | 7.89  | A |
| ATOM | 399 | CG1 | VAL | A | 55 | 21.596 | 45.057 | 25.775 | 1.00 | 7.35  | A |
| ATOM | 400 | CG2 | VAL | A | 55 | 22.229 | 47.518 | 25.707 | 1.00 | 6.23  | A |
| ATOM | 401 | C   | VAL | A | 55 | 19.840 | 45.540 | 23.386 | 1.00 | 9.36  | A |
| ATOM | 402 | O   | VAL | A | 55 | 18.659 | 45.768 | 23.630 | 1.00 | 11.95 | A |
| ATOM | 403 | N   | HIS | A | 56 | 20.258 | 44.441 | 22.755 | 1.00 | 9.82  | A |
| ATOM | 404 | CA  | HIS | A | 56 | 19.323 | 43.432 | 22.285 | 1.00 | 8.89  | A |
| ATOM | 405 | CB  | HIS | A | 56 | 19.552 | 43.218 | 20.782 | 1.00 | 8.33  | A |
| ATOM | 406 | CG  | HIS | A | 56 | 19.455 | 44.485 | 19.985 | 1.00 | 9.48  | A |
| ATOM | 407 | CD2 | HIS | A | 56 | 20.414 | 45.264 | 19.430 | 1.00 | 11.14 | A |
| ATOM | 408 | ND1 | HIS | A | 56 | 18.255 | 45.121 | 19.738 | 1.00 | 13.82 | A |
| ATOM | 409 | CE1 | HIS | A | 56 | 18.483 | 46.236 | 19.064 | 1.00 | 12.14 | A |
| ATOM | 410 | NE2 | HIS | A | 56 | 19.783 | 46.345 | 18.866 | 1.00 | 12.83 | A |
| ATOM | 411 | C   | HIS | A | 56 | 19.389 | 42.097 | 23.033 | 1.00 | 9.87  | A |
| ATOM | 412 | O   | HIS | A | 56 | 18.419 | 41.331 | 23.039 | 1.00 | 8.84  | A |
| ATOM | 413 | N   | TRP | A | 57 | 20.531 | 41.797 | 23.649 | 1.00 | 10.03 | A |
| ATOM | 414 | CA  | TRP | A | 57 | 20.618 | 40.535 | 24.385 | 1.00 | 12.07 | A |
| ATOM | 415 | CB  | TRP | A | 57 | 20.753 | 39.340 | 23.430 | 1.00 | 7.72  | A |
| ATOM | 416 | CG  | TRP | A | 57 | 22.078 | 39.288 | 22.673 | 1.00 | 9.96  | A |
| ATOM | 417 | CD2 | TRP | A | 57 | 23.188 | 38.398 | 22.935 | 1.00 | 8.55  | A |
| ATOM | 418 | CE2 | TRP | A | 57 | 24.161 | 38.642 | 21.945 | 1.00 | 7.37  | A |
| ATOM | 419 | CE3 | TRP | A | 57 | 23.442 | 37.413 | 23.914 | 1.00 | 9.79  | A |
| ATOM | 420 | CD1 | TRP | A | 57 | 22.430 | 40.021 | 21.570 | 1.00 | 9.43  | A |
| ATOM | 421 | NE1 | TRP | A | 57 | 23.685 | 39.637 | 21.124 | 1.00 | 7.89  | A |
| ATOM | 422 | CZ2 | TRP | A | 57 | 25.381 | 37.936 | 21.895 | 1.00 | 8.66  | A |
| ATOM | 423 | CZ3 | TRP | A | 57 | 24.647 | 36.713 | 23.862 | 1.00 | 7.59  | A |
| ATOM | 424 | CH2 | TRP | A | 57 | 25.605 | 36.982 | 22.852 | 1.00 | 13.66 | A |
| ATOM | 425 | C   | TRP | A | 57 | 21.830 | 40.575 | 25.286 | 1.00 | 9.35  | A |
| ATOM | 426 | O   | TRP | A | 57 | 22.648 | 41.481 | 25.179 | 1.00 | 9.06  | A |
| ATOM | 427 | N   | ALA | A | 58 | 21.945 | 39.579 | 26.159 | 1.00 | 6.35  | A |
| ATOM | 428 | CA  | ALA | A | 58 | 23.081 | 39.523 | 27.061 | 1.00 | 8.26  | A |
| ATOM | 429 | CB  | ALA | A | 58 | 22.755 | 40.280 | 28.362 | 1.00 | 10.03 | A |
| ATOM | 430 | C   | ALA | A | 58 | 23.471 | 38.101 | 27.407 | 1.00 | 7.97  | A |
| ATOM | 431 | O   | ALA | A | 58 | 22.638 | 37.207 | 27.401 | 1.00 | 9.27  | A |
| ATOM | 432 | N   | GLY | A | 59 | 24.749 | 37.908 | 27.702 | 1.00 | 9.58  | A |
| ATOM | 433 | CA  | GLY | A | 59 | 25.213 | 36.608 | 28.184 | 1.00 | 7.09  | A |
| ATOM | 434 | C   | GLY | A | 59 | 25.342 | 36.791 | 29.695 | 1.00 | 9.23  | A |
| ATOM | 435 | O   | GLY | A | 59 | 25.779 | 37.846 | 30.159 | 1.00 | 10.14 | A |
| ATOM | 436 | N   | SER | A | 60 | 24.938 | 35.801 | 30.484 | 1.00 | 5.73  | A |
| ATOM | 437 | CA  | SER | A | 60 | 25.058 | 35.917 | 31.938 | 1.00 | 5.95  | A |
| ATOM | 438 | CB  | SER | A | 60 | 23.815 | 36.613 | 32.535 | 1.00 | 10.17 | A |
| ATOM | 439 | OG  | SER | A | 60 | 23.896 | 36.707 | 33.966 | 1.00 | 9.12  | A |
| ATOM | 440 | C   | SER | A | 60 | 25.161 | 34.540 | 32.566 | 1.00 | 8.54  | A |
| ATOM | 441 | O   | SER | A | 60 | 24.437 | 33.632 | 32.146 | 1.00 | 9.12  | A |
| ATOM | 442 | N   | ASP | A | 61 | 26.067 | 34.376 | 33.536 | 1.00 | 9.30  | A |
| ATOM | 443 | CA  | ASP | A | 61 | 26.132 | 33.124 | 34.292 | 1.00 | 8.23  | A |
| ATOM | 444 | CB  | ASP | A | 61 | 27.543 | 32.485 | 34.381 | 1.00 | 6.13  | A |
| ATOM | 445 | CG  | ASP | A | 61 | 28.600 | 33.266 | 33.649 | 1.00 | 13.41 | A |
| ATOM | 446 | OD1 | ASP | A | 61 | 28.869 | 32.961 | 32.449 | 1.00 | 10.15 | A |
| ATOM | 447 | OD2 | ASP | A | 61 | 29.150 | 34.191 | 34.281 | 1.00 | 13.11 | A |
| ATOM | 448 | C   | ASP | A | 61 | 25.597 | 33.456 | 35.710 | 1.00 | 10.77 | A |
| ATOM | 449 | O   | ASP | A | 61 | 25.818 | 32.716 | 36.658 | 1.00 | 11.14 | A |
| ATOM | 450 | N   | SER | A | 62 | 24.914 | 34.595 | 35.833 | 1.00 | 7.59  | A |
| ATOM | 451 | CA  | SER | A | 62 | 24.213 | 34.995 | 37.067 | 1.00 | 10.29 | A |

FIGURE 5 (suite)

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 452 | CB  | SER | A | 62 | 24.522 | 36.437 | 37.497 | 1.00 | 11.42 | A |
| ATOM | 453 | OG  | SER | A | 62 | 23.631 | 36.832 | 38.549 | 1.00 | 11.94 | A |
| ATOM | 454 | C   | SER | A | 62 | 22.721 | 34.944 | 36.706 | 1.00 | 10.70 | A |
| ATOM | 455 | O   | SER | A | 62 | 22.274 | 35.605 | 35.745 | 1.00 | 9.88  | A |
| ATOM | 456 | N   | LYS | A | 63 | 21.944 | 34.168 | 37.449 | 1.00 | 8.95  | A |
| ATOM | 457 | CA  | LYS | A | 63 | 20.519 | 34.089 | 37.137 | 1.00 | 10.67 | A |
| ATOM | 458 | CB  | LYS | A | 63 | 19.834 | 32.996 | 37.959 | 1.00 | 16.43 | A |
| ATOM | 459 | CG  | LYS | A | 63 | 20.046 | 31.605 | 37.461 | 1.00 | 15.34 | A |
| ATOM | 460 | CD  | LYS | A | 63 | 19.148 | 30.619 | 38.201 | 1.00 | 19.94 | A |
| ATOM | 461 | CE  | LYS | A | 63 | 17.702 | 30.671 | 37.728 | 1.00 | 16.96 | A |
| ATOM | 462 | NZ  | LYS | A | 63 | 16.903 | 29.498 | 38.239 | 1.00 | 14.00 | A |
| ATOM | 463 | C   | LYS | A | 63 | 19.786 | 35.392 | 37.399 | 1.00 | 12.40 | A |
| ATOM | 464 | O   | LYS | A | 63 | 20.192 | 36.183 | 38.257 | 1.00 | 10.37 | A |
| ATOM | 465 | N   | LEU | A | 64 | 18.699 | 35.604 | 36.659 | 1.00 | 7.10  | A |
| ATOM | 466 | CA  | LEU | A | 64 | 17.863 | 36.778 | 36.842 | 1.00 | 9.01  | A |
| ATOM | 467 | CB  | LEU | A | 64 | 16.824 | 36.871 | 35.716 | 1.00 | 6.27  | A |
| ATOM | 468 | CG  | LEU | A | 64 | 17.447 | 37.378 | 34.405 | 1.00 | 7.74  | A |
| ATOM | 469 | CD1 | LEU | A | 64 | 16.586 | 37.016 | 33.190 | 1.00 | 8.96  | A |
| ATOM | 470 | CD2 | LEU | A | 64 | 17.619 | 38.883 | 34.510 | 1.00 | 9.78  | A |
| ATOM | 471 | C   | LEU | A | 64 | 17.168 | 36.569 | 38.197 | 1.00 | 10.06 | A |
| ATOM | 472 | O   | LEU | A | 64 | 16.712 | 35.465 | 38.508 | 1.00 | 11.86 | A |
| ATOM | 473 | N   | THR | A | 65 | 17.120 | 37.614 | 39.012 | 1.00 | 6.99  | A |
| ATOM | 474 | CA  | THR | A | 65 | 16.503 | 37.481 | 40.334 | 1.00 | 11.54 | A |
| ATOM | 475 | CB  | THR | A | 65 | 17.097 | 38.472 | 41.341 | 1.00 | 13.33 | A |
| ATOM | 476 | OG1 | THR | A | 65 | 16.736 | 39.811 | 40.952 | 1.00 | 13.29 | A |
| ATOM | 477 | CG2 | THR | A | 65 | 18.644 | 38.331 | 41.395 | 1.00 | 11.42 | A |
| ATOM | 478 | C   | THR | A | 65 | 15.009 | 37.751 | 40.239 | 1.00 | 13.06 | A |
| ATOM | 479 | O   | THR | A | 65 | 14.530 | 38.268 | 39.233 | 1.00 | 9.78  | A |
| ATOM | 480 | N   | ALA | A | 66 | 14.272 | 37.374 | 41.281 | 1.00 | 11.93 | A |
| ATOM | 481 | CA  | ALA | A | 66 | 12.831 | 37.607 | 41.287 | 1.00 | 16.82 | A |
| ATOM | 482 | CB  | ALA | A | 66 | 12.231 | 37.106 | 42.601 | 1.00 | 17.23 | A |
| ATOM | 483 | C   | ALA | A | 66 | 12.527 | 39.104 | 41.105 | 1.00 | 14.69 | A |
| ATOM | 484 | O   | ALA | A | 66 | 11.587 | 39.467 | 40.409 | 1.00 | 12.67 | A |
| ATOM | 485 | N   | SER | A | 67 | 13.322 | 39.962 | 41.744 | 1.00 | 15.98 | A |
| ATOM | 486 | CA  | SER | A | 67 | 13.150 | 41.417 | 41.640 | 1.00 | 12.48 | A |
| ATOM | 487 | CB  | SER | A | 67 | 14.108 | 42.166 | 42.579 | 1.00 | 18.87 | A |
| ATOM | 488 | OG  | SER | A | 67 | 13.662 | 42.081 | 43.921 | 1.00 | 28.18 | A |
| ATOM | 489 | C   | SER | A | 67 | 13.403 | 41.890 | 40.212 | 1.00 | 12.05 | A |
| ATOM | 490 | O   | SER | A | 67 | 12.630 | 42.671 | 39.666 | 1.00 | 12.31 | A |
| ATOM | 491 | N   | GLN | A | 68 | 14.495 | 41.426 | 39.616 | 1.00 | 8.93  | A |
| ATOM | 492 | CA  | GLN | A | 68 | 14.796 | 41.803 | 38.237 | 1.00 | 8.58  | A |
| ATOM | 493 | CB  | GLN | A | 68 | 16.123 | 41.176 | 37.768 | 1.00 | 11.33 | A |
| ATOM | 494 | CG  | GLN | A | 68 | 17.343 | 41.749 | 38.524 | 1.00 | 12.20 | A |
| ATOM | 495 | CD  | GLN | A | 68 | 18.656 | 41.026 | 38.242 | 1.00 | 15.53 | A |
| ATOM | 496 | OE1 | GLN | A | 68 | 18.690 | 39.815 | 38.034 | 1.00 | 11.56 | A |
| ATOM | 497 | NE2 | GLN | A | 68 | 19.743 | 41.770 | 38.255 | 1.00 | 14.33 | A |
| ATOM | 498 | C   | GLN | A | 68 | 13.673 | 41.385 | 37.290 | 1.00 | 12.61 | A |
| ATOM | 499 | O   | GLN | A | 68 | 13.270 | 42.158 | 36.423 | 1.00 | 10.84 | A |
| ATOM | 500 | N   | LEU | A | 69 | 13.163 | 40.164 | 37.455 | 1.00 | 13.81 | A |
| ATOM | 501 | CA  | LEU | A | 69 | 12.093 | 39.687 | 36.576 | 1.00 | 13.47 | A |
| ATOM | 502 | CB  | LEU | A | 69 | 11.809 | 38.189 | 36.829 | 1.00 | 13.08 | A |
| ATOM | 503 | CG  | LEU | A | 69 | 12.989 | 37.268 | 36.496 | 1.00 | 14.83 | A |
| ATOM | 504 | CD1 | LEU | A | 69 | 12.772 | 35.862 | 37.071 | 1.00 | 16.18 | A |
| ATOM | 505 | CD2 | LEU | A | 69 | 13.140 | 37.233 | 34.981 | 1.00 | 11.50 | A |
| ATOM | 506 | C   | LEU | A | 69 | 10.810 | 40.484 | 36.778 | 1.00 | 13.14 | A |
| ATOM | 507 | O   | LEU | A | 69 | 10.138 | 40.860 | 35.814 | 1.00 | 13.07 | A |
| ATOM | 508 | N   | ALA | A | 70 | 10.465 | 40.728 | 38.034 | 1.00 | 12.61 | A |
| ATOM | 509 | CA  | ALA | A | 70 | 9.227  | 41.443 | 38.328 | 1.00 | 12.01 | A |
| ATOM | 510 | CB  | ALA | A | 70 | 8.951  | 41.453 | 39.841 | 1.00 | 13.19 | A |
| ATOM | 511 | C   | ALA | A | 70 | 9.275  | 42.852 | 37.785 | 1.00 | 12.44 | A |
| ATOM | 512 | O   | ALA | A | 70 | 8.297  | 43.334 | 37.240 | 1.00 | 16.48 | A |
| ATOM | 513 | N   | THR | A | 71 | 10.419 | 43.512 | 37.928 | 1.00 | 12.49 | A |
| ATOM | 514 | CA  | THR | A | 71 | 10.574 | 44.865 | 37.436 | 1.00 | 11.47 | A |
| ATOM | 515 | CB  | THR | A | 71 | 11.914 | 45.463 | 37.941 | 1.00 | 18.09 | A |
| ATOM | 516 | OG1 | THR | A | 71 | 11.834 | 45.621 | 39.370 | 1.00 | 19.27 | A |
| ATOM | 517 | CG2 | THR | A | 71 | 12.225 | 46.811 | 37.267 | 1.00 | 13.43 | A |
| ATOM | 518 | C   | THR | A | 71 | 10.501 | 44.905 | 35.902 | 1.00 | 11.57 | A |
| ATOM | 519 | O   | THR | A | 71 | 9.881  | 45.800 | 35.337 | 1.00 | 15.24 | A |
| ATOM | 520 | N   | TYR | A | 72 | 11.116 | 43.941 | 35.223 | 1.00 | 13.13 | A |
| ATOM | 521 | CA  | TYR | A | 72 | 11.049 | 43.941 | 33.760 | 1.00 | 12.95 | A |
| ATOM | 522 | CB  | TYR | A | 72 | 11.927 | 42.839 | 33.174 | 1.00 | 11.21 | A |
| ATOM | 523 | CG  | TYR | A | 72 | 12.194 | 43.011 | 31.682 | 1.00 | 12.14 | A |
| ATOM | 524 | CD1 | TYR | A | 72 | 13.122 | 43.936 | 31.224 | 1.00 | 11.17 | A |
| ATOM | 525 | CE1 | TYR | A | 72 | 13.376 | 44.101 | 29.841 | 1.00 | 11.35 | A |
| ATOM | 526 | CD2 | TYR | A | 72 | 11.515 | 42.239 | 30.736 | 1.00 | 14.03 | A |
| ATOM | 527 | CE2 | TYR | A | 72 | 11.765 | 42.378 | 29.372 | 1.00 | 8.40  | A |

FIGURE 5 (suite)

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 528 | CZ  | TYR | A | 72 | 12.689 | 43.303 | 28.928 | 1.00 | 10.19 | A |
| ATOM | 529 | OH  | TYR | A | 72 | 12.949 | 43.425 | 27.585 | 1.00 | 10.75 | A |
| ATOM | 530 | C   | TYR | A | 72 | 9.604  | 43.705 | 33.313 | 1.00 | 13.42 | A |
| ATOM | 531 | O   | TYR | A | 72 | 9.111  | 44.346 | 32.394 | 1.00 | 14.74 | A |
| ATOM | 532 | N   | ALA | A | 73 | 8.943  | 42.763 | 33.970 | 1.00 | 14.68 | A |
| ATOM | 533 | CA  | ALA | A | 73 | 7.563  | 42.423 | 33.650 | 1.00 | 15.37 | A |
| ATOM | 534 | CB  | ALA | A | 73 | 7.090  | 41.293 | 34.556 | 1.00 | 10.74 | A |
| ATOM | 535 | C   | ALA | A | 73 | 6.631  | 43.626 | 33.791 | 1.00 | 14.04 | A |
| ATOM | 536 | O   | ALA | A | 73 | 5.711  | 43.811 | 32.992 | 1.00 | 13.32 | A |
| ATOM | 537 | N   | ALA | A | 74 | 6.856  | 44.436 | 34.815 | 1.00 | 16.88 | A |
| ATOM | 538 | CA  | ALA | A | 74 | 6.006  | 45.602 | 35.032 | 1.00 | 17.08 | A |
| ATOM | 539 | CB  | ALA | A | 74 | 6.082  | 46.052 | 36.505 | 1.00 | 13.94 | A |
| ATOM | 540 | C   | ALA | A | 74 | 6.354  | 46.768 | 34.118 | 1.00 | 20.94 | A |
| ATOM | 541 | O   | ALA | A | 74 | 5.475  | 47.357 | 33.476 | 1.00 | 17.04 | A |
| ATOM | 542 | N   | ASN | A | 75 | 7.645  | 47.061 | 34.014 | 1.00 | 15.74 | A |
| ATOM | 543 | CA  | ASN | A | 75 | 8.125  | 48.203 | 33.241 | 1.00 | 17.76 | A |
| ATOM | 544 | CB  | ASN | A | 75 | 9.439  | 48.712 | 33.839 | 1.00 | 19.52 | A |
| ATOM | 545 | CG  | ASN | A | 75 | 9.308  | 49.152 | 35.289 | 1.00 | 24.86 | A |
| ATOM | 546 | OD1 | ASN | A | 75 | 10.308 | 49.485 | 35.929 | 1.00 | 26.13 | A |
| ATOM | 547 | ND2 | ASN | A | 75 | 8.084  | 49.150 | 35.816 | 1.00 | 27.41 | A |
| ATOM | 548 | C   | ASN | A | 75 | 8.356  | 48.070 | 31.741 | 1.00 | 18.90 | A |
| ATOM | 549 | O   | ASN | A | 75 | 8.049  | 48.996 | 30.986 | 1.00 | 16.37 | A |
| ATOM | 550 | N   | LYS | A | 76 | 8.910  | 46.944 | 31.304 | 1.00 | 13.20 | A |
| ATOM | 551 | CA  | LYS | A | 76 | 9.235  | 46.810 | 29.888 | 1.00 | 14.05 | A |
| ATOM | 552 | CB  | LYS | A | 76 | 10.709 | 46.412 | 29.730 | 1.00 | 11.81 | A |
| ATOM | 553 | CG  | LYS | A | 76 | 11.706 | 47.189 | 30.561 | 1.00 | 15.12 | A |
| ATOM | 554 | CD  | LYS | A | 76 | 11.710 | 48.673 | 30.208 | 1.00 | 18.17 | A |
| ATOM | 555 | CE  | LYS | A | 76 | 12.942 | 49.342 | 30.783 | 1.00 | 21.75 | A |
| ATOM | 556 | NZ  | LYS | A | 76 | 12.858 | 50.832 | 30.665 | 1.00 | 23.76 | A |
| ATOM | 557 | C   | LYS | A | 76 | 8.414  | 45.835 | 29.064 | 1.00 | 14.89 | A |
| ATOM | 558 | O   | LYS | A | 76 | 8.184  | 46.053 | 27.874 | 1.00 | 15.18 | A |
| ATOM | 559 | N   | GLN | A | 77 | 7.996  | 44.746 | 29.686 | 1.00 | 13.65 | A |
| ATOM | 560 | CA  | GLN | A | 77 | 7.240  | 43.718 | 28.978 | 1.00 | 15.70 | A |
| ATOM | 561 | CB  | GLN | A | 77 | 6.865  | 42.625 | 29.964 | 1.00 | 14.98 | A |
| ATOM | 562 | CG  | GLN | A | 77 | 6.139  | 41.438 | 29.381 | 1.00 | 18.91 | A |
| ATOM | 563 | CD  | GLN | A | 77 | 5.848  | 40.392 | 30.441 | 1.00 | 26.71 | A |
| ATOM | 564 | OE1 | GLN | A | 77 | 6.747  | 39.965 | 31.167 | 1.00 | 25.14 | A |
| ATOM | 565 | NE2 | GLN | A | 77 | 4.593  | 39.968 | 30.534 | 1.00 | 21.79 | A |
| ATOM | 566 | C   | GLN | A | 77 | 5.989  | 44.205 | 28.222 | 1.00 | 16.81 | A |
| ATOM | 567 | O   | GLN | A | 77 | 5.718  | 43.746 | 27.114 | 1.00 | 17.54 | A |
| ATOM | 568 | N   | PRO | A | 78 | 5.216  | 45.142 | 28.800 | 1.00 | 19.48 | A |
| ATOM | 569 | CD  | PRO | A | 78 | 5.255  | 45.765 | 30.134 | 1.00 | 12.68 | A |
| ATOM | 570 | CA  | PRO | A | 78 | 4.023  | 45.575 | 28.056 | 1.00 | 15.54 | A |
| ATOM | 571 | CB  | PRO | A | 78 | 3.428  | 46.654 | 28.958 | 1.00 | 19.25 | A |
| ATOM | 572 | CG  | PRO | A | 78 | 3.787  | 46.150 | 30.342 | 1.00 | 17.82 | A |
| ATOM | 573 | C   | PRO | A | 78 | 4.325  | 46.080 | 26.646 | 1.00 | 20.10 | A |
| ATOM | 574 | O   | PRO | A | 78 | 3.614  | 45.748 | 25.692 | 1.00 | 18.30 | A |
| ATOM | 575 | N   | GLY | A | 79 | 5.393  | 46.860 | 26.512 | 1.00 | 15.27 | A |
| ATOM | 576 | CA  | GLY | A | 79 | 5.745  | 47.379 | 25.210 | 1.00 | 17.02 | A |
| ATOM | 577 | C   | GLY | A | 79 | 6.802  | 46.616 | 24.427 | 1.00 | 20.02 | A |
| ATOM | 578 | O   | GLY | A | 79 | 6.839  | 46.731 | 23.199 | 1.00 | 15.38 | A |
| ATOM | 579 | N   | TRP | A | 80 | 7.639  | 45.830 | 25.111 | 1.00 | 13.75 | A |
| ATOM | 580 | CA  | TRP | A | 80 | 8.723  | 45.092 | 24.440 | 1.00 | 14.43 | A |
| ATOM | 581 | CB  | TRP | A | 80 | 10.052 | 45.359 | 25.136 | 1.00 | 11.39 | A |
| ATOM | 582 | CG  | TRP | A | 80 | 10.549 | 46.780 | 25.071 | 1.00 | 15.13 | A |
| ATOM | 583 | CD2 | TRP | A | 80 | 11.672 | 47.329 | 25.767 | 1.00 | 13.37 | A |
| ATOM | 584 | CE2 | TRP | A | 80 | 11.823 | 48.666 | 25.332 | 1.00 | 13.52 | A |
| ATOM | 585 | CE3 | TRP | A | 80 | 12.573 | 46.817 | 26.716 | 1.00 | 12.51 | A |
| ATOM | 586 | CD1 | TRP | A | 80 | 10.068 | 47.779 | 24.271 | 1.00 | 19.04 | A |
| ATOM | 587 | NE1 | TRP | A | 80 | 10.831 | 48.919 | 24.418 | 1.00 | 16.58 | A |
| ATOM | 588 | CZ2 | TRP | A | 80 | 12.840 | 49.502 | 25.812 | 1.00 | 15.28 | A |
| ATOM | 589 | CZ3 | TRP | A | 80 | 13.586 | 47.645 | 27.197 | 1.00 | 13.05 | A |
| ATOM | 590 | CH2 | TRP | A | 80 | 13.710 | 48.979 | 26.739 | 1.00 | 16.82 | A |
| ATOM | 591 | C   | TRP | A | 80 | 8.560  | 43.580 | 24.349 | 1.00 | 16.83 | A |
| ATOM | 592 | O   | TRP | A | 80 | 9.361  | 42.909 | 23.685 | 1.00 | 16.92 | A |
| ATOM | 593 | N   | GLY | A | 81 | 7.562  | 43.031 | 25.033 | 1.00 | 15.56 | A |
| ATOM | 594 | CA  | GLY | A | 81 | 7.380  | 41.584 | 25.001 | 1.00 | 11.72 | A |
| ATOM | 595 | C   | GLY | A | 81 | 8.071  | 40.921 | 26.186 | 1.00 | 13.05 | A |
| ATOM | 596 | O   | GLY | A | 81 | 8.856  | 41.557 | 26.894 | 1.00 | 8.85  | A |
| ATOM | 597 | N   | LYS | A | 82 | 7.784  | 39.638 | 26.395 | 1.00 | 10.46 | A |
| ATOM | 598 | CA  | LYS | A | 82 | 8.374  | 38.882 | 27.499 | 1.00 | 11.96 | A |
| ATOM | 599 | CB  | LYS | A | 82 | 7.702  | 37.506 | 27.608 | 1.00 | 11.82 | A |
| ATOM | 600 | CG  | LYS | A | 82 | 6.341  | 37.497 | 28.315 | 1.00 | 12.27 | A |
| ATOM | 601 | CD  | LYS | A | 82 | 5.578  | 36.167 | 28.137 | 1.00 | 15.83 | A |
| ATOM | 602 | CE  | LYS | A | 82 | 6.296  | 34.971 | 28.782 | 1.00 | 21.44 | A |
| ATOM | 603 | NZ  | LYS | A | 82 | 6.571  | 35.179 | 30.234 | 1.00 | 18.30 | A |

FIGURE 5 (suite)

|      |     |     |     |   |    |        |        |        |      |       |   |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|---|
| ATOM | 604 | C   | LYS | A | 82 | 9.868  | 38.658 | 27.275 | 1.00 | 12.45 | A |
| ATOM | 605 | O   | LYS | A | 82 | 10.313 | 38.530 | 26.126 | 1.00 | 11.99 | A |
| ATOM | 606 | N   | LEU | A | 83 | 10.649 | 38.598 | 28.357 | 1.00 | 10.87 | A |
| ATOM | 607 | CA  | LEU | A | 83 | 12.057 | 38.305 | 28.161 | 1.00 | 10.47 | A |
| ATOM | 608 | CB  | LEU | A | 83 | 12.955 | 38.929 | 29.248 | 1.00 | 16.59 | A |
| ATOM | 609 | CG  | LEU | A | 83 | 13.059 | 38.501 | 30.707 | 1.00 | 13.98 | A |
| ATOM | 610 | CD1 | LEU | A | 83 | 13.627 | 37.083 | 30.856 | 1.00 | 13.97 | A |
| ATOM | 611 | CD2 | LEU | A | 83 | 14.010 | 39.508 | 31.412 | 1.00 | 12.95 | A |
| ATOM | 612 | C   | LEU | A | 83 | 12.191 | 36.790 | 28.142 | 1.00 | 8.84  | A |
| ATOM | 613 | O   | LEU | A | 83 | 11.288 | 36.062 | 28.604 | 1.00 | 12.14 | A |
| ATOM | 614 | N   | ILE | A | 84 | 13.294 | 36.330 | 27.567 | 1.00 | 9.04  | A |
| ATOM | 615 | CA  | ILE | A | 84 | 13.606 | 34.912 | 27.467 | 1.00 | 7.94  | A |
| ATOM | 616 | CB  | ILE | A | 84 | 13.734 | 34.492 | 25.986 | 1.00 | 11.27 | A |
| ATOM | 617 | CG2 | ILE | A | 84 | 14.322 | 33.075 | 25.875 | 1.00 | 15.02 | A |
| ATOM | 618 | CG1 | ILE | A | 84 | 12.356 | 34.567 | 25.306 | 1.00 | 13.46 | A |
| ATOM | 619 | CD1 | ILE | A | 84 | 12.407 | 34.310 | 23.806 | 1.00 | 10.66 | A |
| ATOM | 620 | C   | ILE | A | 84 | 14.957 | 34.682 | 28.151 | 1.00 | 9.44  | A |
| ATOM | 621 | O   | ILE | A | 84 | 15.918 | 35.410 | 27.891 | 1.00 | 9.33  | A |
| ATOM | 622 | N   | GLU | A | 85 | 15.018 | 33.686 | 29.023 | 1.00 | 7.70  | A |
| ATOM | 623 | CA  | GLU | A | 85 | 16.269 | 33.331 | 29.683 | 1.00 | 8.79  | A |
| ATOM | 624 | CB  | GLU | A | 85 | 16.211 | 33.631 | 31.196 | 1.00 | 7.98  | A |
| ATOM | 625 | CG  | GLU | A | 85 | 17.532 | 33.291 | 31.922 | 1.00 | 8.35  | A |
| ATOM | 626 | CD  | GLU | A | 85 | 17.472 | 33.466 | 33.442 | 1.00 | 9.44  | A |
| ATOM | 627 | OE1 | GLU | A | 85 | 16.520 | 32.969 | 34.103 | 1.00 | 13.35 | A |
| ATOM | 628 | OE2 | GLU | A | 85 | 18.408 | 34.077 | 33.998 | 1.00 | 10.18 | A |
| ATOM | 629 | C   | GLU | A | 85 | 16.452 | 31.832 | 29.442 | 1.00 | 9.15  | A |
| ATOM | 630 | O   | GLU | A | 85 | 15.614 | 31.047 | 29.870 | 1.00 | 10.73 | A |
| ATOM | 631 | N   | VAL | A | 86 | 17.513 | 31.438 | 28.733 | 1.00 | 9.15  | A |
| ATOM | 632 | CA  | VAL | A | 86 | 17.772 | 30.021 | 28.458 | 1.00 | 9.61  | A |
| ATOM | 633 | CB  | VAL | A | 86 | 17.394 | 29.631 | 26.987 | 1.00 | 8.48  | A |
| ATOM | 634 | CG1 | VAL | A | 86 | 15.866 | 29.641 | 26.795 | 1.00 | 11.82 | A |
| ATOM | 635 | CG2 | VAL | A | 86 | 18.062 | 30.587 | 25.998 | 1.00 | 8.25  | A |
| ATOM | 636 | C   | VAL | A | 86 | 19.247 | 29.653 | 28.653 | 1.00 | 12.36 | A |
| ATOM | 637 | O   | VAL | A | 86 | 20.135 | 30.490 | 28.488 | 1.00 | 7.65  | A |
| ATOM | 638 | N   | PRO | A | 87 | 19.530 | 28.392 | 29.034 | 1.00 | 7.50  | A |
| ATOM | 639 | CD  | PRO | A | 87 | 18.611 | 27.261 | 29.245 | 1.00 | 11.19 | A |
| ATOM | 640 | CA  | PRO | A | 87 | 20.927 | 27.986 | 29.213 | 1.00 | 8.03  | A |
| ATOM | 641 | CB  | PRO | A | 87 | 20.806 | 26.551 | 29.747 | 1.00 | 11.47 | A |
| ATOM | 642 | CG  | PRO | A | 87 | 19.531 | 26.065 | 29.123 | 1.00 | 18.08 | A |
| ATOM | 643 | C   | PRO | A | 87 | 21.551 | 28.031 | 27.803 | 1.00 | 12.05 | A |
| ATOM | 644 | O   | PRO | A | 87 | 20.845 | 27.799 | 26.798 | 1.00 | 11.64 | A |
| ATOM | 645 | N   | SER | A | 88 | 22.844 | 28.346 | 27.739 | 1.00 | 10.05 | A |
| ATOM | 646 | CA  | SER | A | 88 | 23.607 | 28.427 | 26.480 | 1.00 | 8.91  | A |
| ATOM | 647 | CB  | SER | A | 88 | 24.472 | 29.695 | 26.471 | 1.00 | 6.92  | A |
| ATOM | 648 | OG  | SER | A | 88 | 25.266 | 29.787 | 25.294 | 1.00 | 11.36 | A |
| ATOM | 649 | C   | SER | A | 88 | 24.484 | 27.177 | 26.379 | 1.00 | 7.85  | A |
| ATOM | 650 | O   | SER | A | 88 | 24.385 | 26.432 | 25.401 | 1.00 | 7.71  | A |
| ATOM | 651 | N   | VAL | A | 89 | 25.365 | 26.993 | 27.368 | 1.00 | 7.73  | A |
| ATOM | 652 | CA  | VAL | A | 89 | 26.218 | 25.802 | 27.481 | 1.00 | 8.66  | A |
| ATOM | 653 | CB  | VAL | A | 89 | 27.639 | 26.010 | 26.874 | 1.00 | 5.11  | A |
| ATOM | 654 | CG1 | VAL | A | 89 | 27.522 | 26.503 | 25.400 | 1.00 | 7.72  | A |
| ATOM | 655 | CG2 | VAL | A | 89 | 28.444 | 27.016 | 27.744 | 1.00 | 8.02  | A |
| ATOM | 656 | C   | VAL | A | 89 | 26.407 | 25.527 | 28.980 | 1.00 | 10.90 | A |
| ATOM | 657 | O   | VAL | A | 89 | 26.037 | 26.356 | 29.809 | 1.00 | 9.82  | A |
| ATOM | 658 | N   | ALA | A | 90 | 26.982 | 24.369 | 29.325 | 1.00 | 10.64 | A |
| ATOM | 659 | CA  | ALA | A | 90 | 27.242 | 24.059 | 30.722 | 1.00 | 8.29  | A |
| ATOM | 660 | CB  | ALA | A | 90 | 26.792 | 22.616 | 31.077 | 1.00 | 8.16  | A |
| ATOM | 661 | C   | ALA | A | 90 | 28.764 | 24.190 | 30.863 | 1.00 | 7.63  | A |
| ATOM | 662 | O   | ALA | A | 90 | 29.498 | 24.095 | 29.880 | 1.00 | 7.66  | A |
| ATOM | 663 | N   | THR | A | 91 | 29.233 | 24.345 | 32.091 | 1.00 | 7.77  | A |
| ATOM | 664 | CA  | THR | A | 91 | 30.651 | 24.559 | 32.300 | 1.00 | 9.18  | A |
| ATOM | 665 | CB  | THR | A | 91 | 30.945 | 26.074 | 32.165 | 1.00 | 10.09 | A |
| ATOM | 666 | OG1 | THR | A | 91 | 32.337 | 26.323 | 32.365 | 1.00 | 11.79 | A |
| ATOM | 667 | CG2 | THR | A | 91 | 30.156 | 26.862 | 33.214 | 1.00 | 11.41 | A |
| ATOM | 668 | C   | THR | A | 91 | 31.116 | 24.140 | 33.686 | 1.00 | 10.91 | A |
| ATOM | 669 | O   | THR | A | 91 | 30.326 | 24.055 | 34.614 | 1.00 | 9.96  | A |
| ATOM | 670 | N   | SER | A | 92 | 32.409 | 23.858 | 33.811 | 1.00 | 11.52 | A |
| ATOM | 671 | CA  | SER | A | 92 | 32.972 | 23.598 | 35.122 | 1.00 | 9.75  | A |
| ATOM | 672 | CB  | SER | A | 92 | 34.167 | 22.642 | 35.011 | 1.00 | 12.03 | A |
| ATOM | 673 | OG  | SER | A | 92 | 35.213 | 23.181 | 34.186 | 1.00 | 10.62 | A |
| ATOM | 674 | C   | SER | A | 92 | 33.490 | 24.962 | 35.601 | 1.00 | 10.73 | A |
| ATOM | 675 | O   | SER | A | 92 | 33.397 | 25.974 | 34.883 | 1.00 | 8.53  | A |
| ATOM | 676 | N   | VAL | A | 93 | 33.980 | 25.003 | 36.837 | 1.00 | 8.68  | A |
| ATOM | 677 | CA  | VAL | A | 93 | 34.640 | 26.197 | 37.369 | 1.00 | 7.08  | A |
| ATOM | 678 | CB  | VAL | A | 93 | 34.010 | 26.736 | 38.667 | 1.00 | 7.09  | A |
| ATOM | 679 | CG1 | VAL | A | 93 | 34.896 | 27.906 | 39.215 | 1.00 | 10.40 | A |

FIGURE 5 (suite)

|      |     |     |       |     |        |        |        |      |       |   |
|------|-----|-----|-------|-----|--------|--------|--------|------|-------|---|
| ATOM | 680 | CG2 | VAL A | 93  | 32.592 | 27.269 | 38.376 | 1.00 | 10.45 | A |
| ATOM | 681 | C   | VAL A | 93  | 36.033 | 25.643 | 37.694 | 1.00 | 9.49  | A |
| ATOM | 682 | O   | VAL A | 93  | 36.162 | 24.745 | 38.527 | 1.00 | 12.26 | A |
| ATOM | 683 | N   | ALA A | 94  | 37.064 | 26.148 | 37.025 | 1.00 | 8.00  | A |
| ATOM | 684 | CA  | ALA A | 94  | 38.425 | 25.645 | 37.236 | 1.00 | 8.64  | A |
| ATOM | 685 | CB  | ALA A | 94  | 39.204 | 25.722 | 35.921 | 1.00 | 7.88  | A |
| ATOM | 686 | C   | ALA A | 94  | 39.197 | 26.374 | 38.329 | 1.00 | 7.97  | A |
| ATOM | 687 | O   | ALA A | 94  | 38.906 | 27.530 | 38.625 | 1.00 | 8.61  | A |
| ATOM | 688 | N   | ILE A | 95  | 40.210 | 25.709 | 38.894 | 1.00 | 5.77  | A |
| ATOM | 689 | CA  | ILE A | 95  | 41.016 | 26.290 | 39.963 | 1.00 | 7.30  | A |
| ATOM | 690 | CB  | ILE A | 95  | 40.870 | 25.486 | 41.307 | 1.00 | 9.66  | A |
| ATOM | 691 | CG2 | ILE A | 95  | 41.522 | 26.261 | 42.465 | 1.00 | 6.29  | A |
| ATOM | 692 | CG1 | ILE A | 95  | 39.401 | 25.218 | 41.641 | 1.00 | 10.13 | A |
| ATOM | 693 | CD1 | ILE A | 95  | 38.566 | 26.491 | 41.909 | 1.00 | 13.60 | A |
| ATOM | 694 | C   | ILE A | 95  | 42.496 | 26.263 | 39.572 | 1.00 | 8.10  | A |
| ATOM | 695 | O   | ILE A | 95  | 43.261 | 25.373 | 40.001 | 1.00 | 10.23 | A |
| ATOM | 696 | N   | PRO A | 96  | 42.923 | 27.216 | 38.742 | 1.00 | 6.65  | A |
| ATOM | 697 | CD  | PRO A | 96  | 42.133 | 28.263 | 38.063 | 1.00 | 6.16  | A |
| ATOM | 698 | CA  | PRO A | 96  | 44.330 | 27.265 | 38.326 | 1.00 | 7.43  | A |
| ATOM | 699 | CB  | PRO A | 96  | 44.275 | 28.107 | 37.054 | 1.00 | 9.06  | A |
| ATOM | 700 | CG  | PRO A | 96  | 43.207 | 29.147 | 37.446 | 1.00 | 8.84  | A |
| ATOM | 701 | C   | PRO A | 96  | 45.133 | 27.938 | 39.434 | 1.00 | 10.94 | A |
| ATOM | 702 | O   | PRO A | 96  | 44.574 | 28.645 | 40.277 | 1.00 | 8.21  | A |
| ATOM | 703 | N   | PHE A | 97  | 46.441 | 27.715 | 39.447 | 1.00 | 9.05  | A |
| ATOM | 704 | CA  | PHE A | 97  | 47.276 | 28.302 | 40.480 | 1.00 | 8.97  | A |
| ATOM | 705 | CB  | PHE A | 97  | 47.259 | 27.414 | 41.732 | 1.00 | 10.70 | A |
| ATOM | 706 | CG  | PHE A | 97  | 47.748 | 26.015 | 41.477 | 1.00 | 9.86  | A |
| ATOM | 707 | CD1 | PHE A | 97  | 49.114 | 25.720 | 41.524 | 1.00 | 10.13 | A |
| ATOM | 708 | CD2 | PHE A | 97  | 46.862 | 25.010 | 41.121 | 1.00 | 7.97  | A |
| ATOM | 709 | CE1 | PHE A | 97  | 49.589 | 24.436 | 41.211 | 1.00 | 9.97  | A |
| ATOM | 710 | CE2 | PHE A | 97  | 47.326 | 23.704 | 40.802 | 1.00 | 8.94  | A |
| ATOM | 711 | CZ  | PHE A | 97  | 48.709 | 23.433 | 40.852 | 1.00 | 7.63  | A |
| ATOM | 712 | C   | PHE A | 97  | 48.698 | 28.418 | 39.949 | 1.00 | 9.55  | A |
| ATOM | 713 | O   | PHE A | 97  | 49.054 | 27.761 | 38.962 | 1.00 | 9.51  | A |
| ATOM | 714 | N   | ARG A | 98  | 49.498 | 29.260 | 40.597 | 1.00 | 8.26  | A |
| ATOM | 715 | CA  | ARG A | 98  | 50.900 | 29.457 | 40.205 | 1.00 | 11.26 | A |
| ATOM | 716 | CB  | ARG A | 98  | 51.149 | 30.927 | 39.808 | 1.00 | 13.41 | A |
| ATOM | 717 | CG  | ARG A | 98  | 52.624 | 31.218 | 39.452 | 1.00 | 12.41 | A |
| ATOM | 718 | CD  | ARG A | 98  | 52.902 | 32.648 | 39.002 | 1.00 | 15.00 | A |
| ATOM | 719 | NE  | ARG A | 98  | 54.350 | 32.871 | 38.907 | 1.00 | 20.95 | A |
| ATOM | 720 | CZ  | ARG A | 98  | 55.048 | 33.714 | 39.670 | 1.00 | 19.61 | A |
| ATOM | 721 | NH1 | ARG A | 98  | 54.454 | 34.446 | 40.606 | 1.00 | 16.05 | A |
| ATOM | 722 | NH2 | ARG A | 98  | 56.361 | 33.824 | 39.500 | 1.00 | 22.95 | A |
| ATOM | 723 | C   | ARG A | 98  | 51.765 | 29.079 | 41.415 | 1.00 | 9.82  | A |
| ATOM | 724 | O   | ARG A | 98  | 51.955 | 29.881 | 42.327 | 1.00 | 12.72 | A |
| ATOM | 725 | N   | LYS A | 99  | 52.258 | 27.838 | 41.417 | 1.00 | 13.72 | A |
| ATOM | 726 | CA  | LYS A | 99  | 53.081 | 27.314 | 42.510 | 1.00 | 14.88 | A |
| ATOM | 727 | CB  | LYS A | 99  | 52.179 | 26.922 | 43.688 | 1.00 | 10.80 | A |
| ATOM | 728 | CG  | LYS A | 99  | 52.899 | 26.401 | 44.919 | 1.00 | 8.32  | A |
| ATOM | 729 | CD  | LYS A | 99  | 53.744 | 27.518 | 45.557 | 1.00 | 10.62 | A |
| ATOM | 730 | CE  | LYS A | 99  | 54.525 | 27.007 | 46.790 | 1.00 | 10.76 | A |
| ATOM | 731 | NZ  | LYS A | 99  | 55.346 | 28.125 | 47.368 | 1.00 | 13.56 | A |
| ATOM | 732 | C   | LYS A | 99  | 53.809 | 26.095 | 41.956 | 1.00 | 14.43 | A |
| ATOM | 733 | O   | LYS A | 99  | 53.200 | 25.056 | 41.701 | 1.00 | 15.34 | A |
| ATOM | 734 | N   | ALA A | 100 | 55.120 | 26.226 | 41.769 | 1.00 | 12.67 | A |
| ATOM | 735 | CA  | ALA A | 100 | 55.911 | 25.143 | 41.202 | 1.00 | 14.53 | A |
| ATOM | 736 | CB  | ALA A | 100 | 57.354 | 25.629 | 40.914 | 1.00 | 14.12 | A |
| ATOM | 737 | C   | ALA A | 100 | 55.960 | 23.900 | 42.072 | 1.00 | 14.42 | A |
| ATOM | 738 | O   | ALA A | 100 | 55.929 | 23.987 | 43.303 | 1.00 | 16.53 | A |
| ATOM | 739 | N   | GLY A | 101 | 56.061 | 22.751 | 41.409 | 1.00 | 10.16 | A |
| ATOM | 740 | CA  | GLY A | 101 | 56.133 | 21.476 | 42.096 | 1.00 | 11.78 | A |
| ATOM | 741 | C   | GLY A | 101 | 55.786 | 20.360 | 41.136 | 1.00 | 17.78 | A |
| ATOM | 742 | O   | GLY A | 101 | 54.853 | 20.479 | 40.338 | 1.00 | 14.78 | A |
| ATOM | 743 | N   | GLY A | 102 | 56.543 | 19.274 | 41.195 | 1.00 | 13.81 | A |
| ATOM | 744 | CA  | GLY A | 102 | 56.273 | 18.156 | 40.313 | 1.00 | 20.81 | A |
| ATOM | 745 | C   | GLY A | 102 | 55.051 | 17.348 | 40.720 | 1.00 | 16.58 | A |
| ATOM | 746 | O   | GLY A | 102 | 54.498 | 16.627 | 39.898 | 1.00 | 16.24 | A |
| ATOM | 747 | N   | ASN A | 103 | 54.624 | 17.451 | 41.976 | 1.00 | 17.72 | A |
| ATOM | 748 | CA  | ASN A | 103 | 53.465 | 16.675 | 42.434 | 1.00 | 16.85 | A |
| ATOM | 749 | CB  | ASN A | 103 | 53.372 | 16.694 | 43.963 | 1.00 | 15.22 | A |
| ATOM | 750 | CG  | ASN A | 103 | 54.365 | 15.760 | 44.615 | 1.00 | 23.02 | A |
| ATOM | 751 | OD1 | ASN A | 103 | 55.279 | 15.249 | 43.955 | 1.00 | 19.32 | A |
| ATOM | 752 | ND2 | ASN A | 103 | 54.205 | 15.535 | 45.916 | 1.00 | 15.75 | A |
| ATOM | 753 | C   | ASN A | 103 | 52.145 | 17.197 | 41.885 | 1.00 | 15.38 | A |
| ATOM | 754 | O   | ASN A | 103 | 51.991 | 18.390 | 41.666 | 1.00 | 11.02 | A |
| ATOM | 755 | N   | ALA A | 104 | 51.183 | 16.306 | 41.693 | 1.00 | 16.02 | A |

FIGURE 5 (suite)

|      |     |     |           |        |        |        |      |       |   |
|------|-----|-----|-----------|--------|--------|--------|------|-------|---|
| ATOM | 756 | CA  | ALA A 104 | 49.880 | 16.744 | 41.219 | 1.00 | 16.65 | A |
| ATOM | 757 | CB  | ALA A 104 | 49.068 | 15.538 | 40.741 | 1.00 | 20.27 | A |
| ATOM | 758 | C   | ALA A 104 | 49.170 | 17.427 | 42.395 | 1.00 | 15.98 | A |
| ATOM | 759 | O   | ALA A 104 | 49.298 | 16.986 | 43.531 | 1.00 | 15.25 | A |
| ATOM | 760 | N   | VAL A 105 | 48.470 | 18.530 | 42.127 | 1.00 | 13.62 | A |
| ATOM | 761 | CA  | VAL A 105 | 47.701 | 19.227 | 43.157 | 1.00 | 13.77 | A |
| ATOM | 762 | CB  | VAL A 105 | 47.708 | 20.756 | 42.945 | 1.00 | 15.80 | A |
| ATOM | 763 | CG1 | VAL A 105 | 46.645 | 21.409 | 43.814 | 1.00 | 16.24 | A |
| ATOM | 764 | CG2 | VAL A 105 | 49.081 | 21.310 | 43.295 | 1.00 | 15.48 | A |
| ATOM | 765 | C   | VAL A 105 | 46.273 | 18.699 | 43.026 | 1.00 | 13.93 | A |
| ATOM | 766 | O   | VAL A 105 | 45.634 | 18.867 | 41.982 | 1.00 | 11.00 | A |
| ATOM | 767 | N   | ASP A 106 | 45.781 | 18.059 | 44.085 | 1.00 | 11.30 | A |
| ATOM | 768 | CA  | ASP A 106 | 44.446 | 17.447 | 44.087 | 1.00 | 13.33 | A |
| ATOM | 769 | CB  | ASP A 106 | 44.594 | 15.914 | 44.007 | 1.00 | 15.23 | A |
| ATOM | 770 | CG  | ASP A 106 | 43.266 | 15.181 | 43.763 | 1.00 | 18.75 | A |
| ATOM | 771 | OD1 | ASP A 106 | 43.294 | 13.932 | 43.636 | 1.00 | 20.08 | A |
| ATOM | 772 | OD2 | ASP A 106 | 42.201 | 15.832 | 43.705 | 1.00 | 16.37 | A |
| ATOM | 773 | C   | ASP A 106 | 43.748 | 17.854 | 45.371 | 1.00 | 13.44 | A |
| ATOM | 774 | O   | ASP A 106 | 44.013 | 17.312 | 46.441 | 1.00 | 12.47 | A |
| ATOM | 775 | N   | LEU A 107 | 42.838 | 18.809 | 45.256 | 1.00 | 12.47 | A |
| ATOM | 776 | CA  | LEU A 107 | 42.126 | 19.322 | 46.424 | 1.00 | 10.60 | A |
| ATOM | 777 | CB  | LEU A 107 | 41.608 | 20.743 | 46.139 | 1.00 | 9.94  | A |
| ATOM | 778 | CG  | LEU A 107 | 42.656 | 21.830 | 45.874 | 1.00 | 15.11 | A |
| ATOM | 779 | CD1 | LEU A 107 | 41.992 | 23.049 | 45.233 | 1.00 | 12.77 | A |
| ATOM | 780 | CD2 | LEU A 107 | 43.332 | 22.222 | 47.191 | 1.00 | 15.50 | A |
| ATOM | 781 | C   | LEU A 107 | 40.936 | 18.504 | 46.860 | 1.00 | 11.58 | A |
| ATOM | 782 | O   | LEU A 107 | 40.118 | 18.134 | 46.029 | 1.00 | 11.26 | A |
| ATOM | 783 | N   | SER A 108 | 40.840 | 18.205 | 48.157 | 1.00 | 10.03 | A |
| ATOM | 784 | CA  | SER A 108 | 39.632 | 17.555 | 48.632 | 1.00 | 9.49  | A |
| ATOM | 785 | CB  | SER A 108 | 39.823 | 16.938 | 50.026 | 1.00 | 11.45 | A |
| ATOM | 786 | OG  | SER A 108 | 40.112 | 17.944 | 50.988 | 1.00 | 10.62 | A |
| ATOM | 787 | C   | SER A 108 | 38.685 | 18.762 | 48.734 | 1.00 | 13.88 | A |
| ATOM | 788 | O   | SER A 108 | 39.137 | 19.909 | 48.733 | 1.00 | 9.31  | A |
| ATOM | 789 | N   | VAL A 109 | 37.384 | 18.528 | 48.795 | 1.00 | 11.62 | A |
| ATOM | 790 | CA  | VAL A 109 | 36.456 | 19.648 | 48.915 | 1.00 | 12.52 | A |
| ATOM | 791 | CB  | VAL A 109 | 34.997 | 19.149 | 48.822 | 1.00 | 14.25 | A |
| ATOM | 792 | CG1 | VAL A 109 | 34.022 | 20.273 | 49.172 | 1.00 | 10.43 | A |
| ATOM | 793 | CG2 | VAL A 109 | 34.738 | 18.624 | 47.385 | 1.00 | 9.95  | A |
| ATOM | 794 | C   | VAL A 109 | 36.705 | 20.397 | 50.228 | 1.00 | 8.60  | A |
| ATOM | 795 | O   | VAL A 109 | 36.646 | 21.622 | 50.265 | 1.00 | 9.21  | A |
| ATOM | 796 | N   | LYS A 110 | 36.995 | 19.666 | 51.301 | 1.00 | 9.28  | A |
| ATOM | 797 | CA  | LYS A 110 | 37.307 | 20.305 | 52.593 | 1.00 | 7.04  | A |
| ATOM | 798 | CB  | LYS A 110 | 37.597 | 19.237 | 53.650 | 1.00 | 7.60  | A |
| ATOM | 799 | CG  | LYS A 110 | 38.038 | 19.793 | 55.030 | 1.00 | 9.51  | A |
| ATOM | 800 | CD  | LYS A 110 | 36.987 | 20.726 | 55.655 | 1.00 | 7.71  | A |
| ATOM | 801 | CE  | LYS A 110 | 37.436 | 21.170 | 57.033 | 1.00 | 15.09 | A |
| ATOM | 802 | NZ  | LYS A 110 | 36.482 | 22.129 | 57.688 | 1.00 | 11.10 | A |
| ATOM | 803 | C   | LYS A 110 | 38.532 | 21.234 | 52.452 | 1.00 | 8.55  | A |
| ATOM | 804 | O   | LYS A 110 | 38.588 | 22.313 | 53.040 | 1.00 | 9.65  | A |
| ATOM | 805 | N   | GLU A 111 | 39.530 | 20.803 | 51.696 | 1.00 | 8.56  | A |
| ATOM | 806 | CA  | GLU A 111 | 40.711 | 21.640 | 51.495 | 1.00 | 11.39 | A |
| ATOM | 807 | CB  | GLU A 111 | 41.817 | 20.836 | 50.800 | 1.00 | 13.45 | A |
| ATOM | 808 | CG  | GLU A 111 | 42.582 | 19.940 | 51.784 | 1.00 | 15.25 | A |
| ATOM | 809 | CD  | GLU A 111 | 43.527 | 18.960 | 51.098 | 1.00 | 16.99 | A |
| ATOM | 810 | OE1 | GLU A 111 | 44.310 | 18.296 | 51.808 | 1.00 | 12.70 | A |
| ATOM | 811 | OE2 | GLU A 111 | 43.477 | 18.851 | 49.860 | 1.00 | 13.80 | A |
| ATOM | 812 | C   | GLU A 111 | 40.342 | 22.881 | 50.663 | 1.00 | 12.16 | A |
| ATOM | 813 | O   | GLU A 111 | 40.751 | 23.998 | 50.983 | 1.00 | 8.45  | A |
| ATOM | 814 | N   | LEU A 112 | 39.586 | 22.680 | 49.587 | 1.00 | 11.50 | A |
| ATOM | 815 | CA  | LEU A 112 | 39.157 | 23.802 | 48.753 | 1.00 | 11.60 | A |
| ATOM | 816 | CB  | LEU A 112 | 38.127 | 23.339 | 47.728 | 1.00 | 12.29 | A |
| ATOM | 817 | CG  | LEU A 112 | 37.520 | 24.486 | 46.906 | 1.00 | 13.68 | A |
| ATOM | 818 | CD1 | LEU A 112 | 38.486 | 24.835 | 45.793 | 1.00 | 14.87 | A |
| ATOM | 819 | CD2 | LEU A 112 | 36.183 | 24.067 | 46.307 | 1.00 | 23.81 | A |
| ATOM | 820 | C   | LEU A 112 | 38.491 | 24.845 | 49.648 | 1.00 | 11.64 | A |
| ATOM | 821 | O   | LEU A 112 | 38.782 | 26.036 | 49.569 | 1.00 | 9.35  | A |
| ATOM | 822 | N   | CYS A 113 | 37.598 | 24.370 | 50.511 | 1.00 | 9.13  | A |
| ATOM | 823 | CA  | CYS A 113 | 36.869 | 25.251 | 51.407 | 1.00 | 10.02 | A |
| ATOM | 824 | C   | CYS A 113 | 37.806 | 26.040 | 52.332 | 1.00 | 10.42 | A |
| ATOM | 825 | O   | CYS A 113 | 37.620 | 27.243 | 52.550 | 1.00 | 9.94  | A |
| ATOM | 826 | CB  | CYS A 113 | 35.881 | 24.414 | 52.215 | 1.00 | 7.06  | A |
| ATOM | 827 | SG  | CYS A 113 | 34.495 | 23.714 | 51.225 | 1.00 | 12.97 | A |
| ATOM | 828 | N   | GLY A 114 | 38.815 | 25.357 | 52.854 | 1.00 | 8.53  | A |
| ATOM | 829 | CA  | GLY A 114 | 39.774 | 25.979 | 53.746 | 1.00 | 8.15  | A |
| ATOM | 830 | C   | GLY A 114 | 40.615 | 27.023 | 53.048 | 1.00 | 8.58  | A |
| ATOM | 831 | O   | GLY A 114 | 40.974 | 28.045 | 53.660 | 1.00 | 9.42  | A |

FIGURE 5 (suite)

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 832 | N   | VAL | A | 115 | 40.929 | 26.780 | 51.773 | 1.00 | 8.91  | A |
| ATOM | 833 | CA  | VAL | A | 115 | 41.724 | 27.727 | 51.001 | 1.00 | 11.99 | A |
| ATOM | 834 | CB  | VAL | A | 115 | 42.142 | 27.154 | 49.611 | 1.00 | 10.97 | A |
| ATOM | 835 | CG1 | VAL | A | 115 | 42.754 | 28.274 | 48.736 | 1.00 | 12.08 | A |
| ATOM | 836 | CG2 | VAL | A | 115 | 43.175 | 26.034 | 49.794 | 1.00 | 9.96  | A |
| ATOM | 837 | C   | VAL | A | 115 | 40.933 | 28.999 | 50.769 | 1.00 | 10.50 | A |
| ATOM | 838 | O   | VAL | A | 115 | 41.450 | 30.107 | 50.958 | 1.00 | 10.53 | A |
| ATOM | 839 | N   | PHE | A | 116 | 39.672 | 28.856 | 50.383 | 1.00 | 10.04 | A |
| ATOM | 840 | CA  | PHE | A | 116 | 38.885 | 30.046 | 50.123 | 1.00 | 12.53 | A |
| ATOM | 841 | CB  | PHE | A | 116 | 37.891 | 29.774 | 49.000 | 1.00 | 8.51  | A |
| ATOM | 842 | CG  | PHE | A | 116 | 38.564 | 29.656 | 47.664 | 1.00 | 8.77  | A |
| ATOM | 843 | CD1 | PHE | A | 116 | 39.041 | 28.429 | 47.220 | 1.00 | 7.52  | A |
| ATOM | 844 | CD2 | PHE | A | 116 | 38.792 | 30.791 | 46.892 | 1.00 | 10.79 | A |
| ATOM | 845 | CE1 | PHE | A | 116 | 39.742 | 28.319 | 46.019 | 1.00 | 11.26 | A |
| ATOM | 846 | CE2 | PHE | A | 116 | 39.494 | 30.708 | 45.682 | 1.00 | 12.98 | A |
| ATOM | 847 | CZ  | PHE | A | 116 | 39.971 | 29.463 | 45.244 | 1.00 | 12.19 | A |
| ATOM | 848 | C   | PHE | A | 116 | 38.236 | 30.713 | 51.319 | 1.00 | 11.72 | A |
| ATOM | 849 | O   | PHE | A | 116 | 37.688 | 31.802 | 51.180 | 1.00 | 10.01 | A |
| ATOM | 850 | N   | SER | A | 117 | 38.323 | 30.077 | 52.493 | 1.00 | 7.36  | A |
| ATOM | 851 | CA  | SER | A | 117 | 37.802 | 30.669 | 53.722 | 1.00 | 12.12 | A |
| ATOM | 852 | CB  | SER | A | 117 | 37.217 | 29.605 | 54.654 | 1.00 | 11.41 | A |
| ATOM | 853 | OG  | SER | A | 117 | 38.251 | 28.827 | 55.231 | 1.00 | 12.73 | A |
| ATOM | 854 | C   | SER | A | 117 | 38.935 | 31.372 | 54.474 | 1.00 | 12.93 | A |
| ATOM | 855 | O   | SER | A | 117 | 38.693 | 32.241 | 55.316 | 1.00 | 9.90  | A |
| ATOM | 856 | N   | GLY | A | 118 | 40.169 | 30.988 | 54.174 | 1.00 | 14.10 | A |
| ATOM | 857 | CA  | GLY | A | 118 | 41.312 | 31.576 | 54.860 | 1.00 | 13.07 | A |
| ATOM | 858 | C   | GLY | A | 118 | 41.850 | 30.640 | 55.931 | 1.00 | 15.32 | A |
| ATOM | 859 | O   | GLY | A | 118 | 42.935 | 30.873 | 56.484 | 1.00 | 15.65 | A |
| ATOM | 860 | N   | ARG | A | 119 | 41.107 | 29.575 | 56.241 | 1.00 | 15.32 | A |
| ATOM | 861 | CA  | ARG | A | 119 | 41.550 | 28.622 | 57.266 | 1.00 | 15.10 | A |
| ATOM | 862 | CB  | ARG | A | 119 | 40.503 | 27.518 | 57.485 | 1.00 | 17.52 | A |
| ATOM | 863 | CG  | ARG | A | 119 | 40.986 | 26.359 | 58.390 | 1.00 | 19.04 | A |
| ATOM | 864 | CD  | ARG | A | 119 | 39.880 | 25.325 | 58.628 | 1.00 | 17.23 | A |
| ATOM | 865 | NE  | ARG | A | 119 | 39.338 | 24.771 | 57.377 | 1.00 | 11.41 | A |
| ATOM | 866 | CZ  | ARG | A | 119 | 39.828 | 23.717 | 56.727 | 1.00 | 13.77 | A |
| ATOM | 867 | NH1 | ARG | A | 119 | 40.895 | 23.061 | 57.188 | 1.00 | 9.19  | A |
| ATOM | 868 | NH2 | ARG | A | 119 | 39.239 | 23.317 | 55.607 | 1.00 | 10.56 | A |
| ATOM | 869 | C   | ARG | A | 119 | 42.896 | 27.990 | 56.896 | 1.00 | 14.09 | A |
| ATOM | 870 | O   | ARG | A | 119 | 43.749 | 27.784 | 57.757 | 1.00 | 12.49 | A |
| ATOM | 871 | N   | ILE | A | 120 | 43.074 | 27.672 | 55.620 | 1.00 | 14.25 | A |
| ATOM | 872 | CA  | ILE | A | 120 | 44.327 | 27.088 | 55.134 | 1.00 | 11.87 | A |
| ATOM | 873 | CB  | ILE | A | 120 | 44.066 | 25.956 | 54.113 | 1.00 | 13.86 | A |
| ATOM | 874 | CG2 | ILE | A | 120 | 45.373 | 25.443 | 53.529 | 1.00 | 12.88 | A |
| ATOM | 875 | CG1 | ILE | A | 120 | 43.349 | 24.796 | 54.812 | 1.00 | 12.97 | A |
| ATOM | 876 | CD1 | ILE | A | 120 | 42.920 | 23.638 | 53.863 | 1.00 | 12.93 | A |
| ATOM | 877 | C   | ILE | A | 120 | 45.042 | 28.241 | 54.445 | 1.00 | 16.50 | A |
| ATOM | 878 | O   | ILE | A | 120 | 44.606 | 28.704 | 53.391 | 1.00 | 15.43 | A |
| ATOM | 879 | N   | ALA | A | 121 | 46.131 | 28.706 | 55.051 | 1.00 | 15.30 | A |
| ATOM | 880 | CA  | ALA | A | 121 | 46.884 | 29.848 | 54.529 | 1.00 | 14.70 | A |
| ATOM | 881 | CB  | ALA | A | 121 | 47.111 | 30.850 | 55.640 | 1.00 | 21.39 | A |
| ATOM | 882 | C   | ALA | A | 121 | 48.211 | 29.482 | 53.904 | 1.00 | 15.45 | A |
| ATOM | 883 | O   | ALA | A | 121 | 48.868 | 30.329 | 53.284 | 1.00 | 16.44 | A |
| ATOM | 884 | N   | ASN | A | 122 | 48.608 | 28.227 | 54.056 | 1.00 | 12.07 | A |
| ATOM | 885 | CA  | ASN | A | 122 | 49.887 | 27.789 | 53.507 | 1.00 | 12.53 | A |
| ATOM | 886 | CB  | ASN | A | 122 | 50.853 | 27.467 | 54.660 | 1.00 | 13.64 | A |
| ATOM | 887 | CG  | ASN | A | 122 | 52.279 | 27.293 | 54.188 | 1.00 | 16.68 | A |
| ATOM | 888 | OD1 | ASN | A | 122 | 52.666 | 26.224 | 53.725 | 1.00 | 18.01 | A |
| ATOM | 889 | ND2 | ASN | A | 122 | 53.063 | 28.363 | 54.279 | 1.00 | 14.68 | A |
| ATOM | 890 | C   | ASN | A | 122 | 49.681 | 26.568 | 52.608 | 1.00 | 11.32 | A |
| ATOM | 891 | O   | ASN | A | 122 | 48.809 | 25.737 | 52.865 | 1.00 | 11.94 | A |
| ATOM | 892 | N   | TRP | A | 123 | 50.454 | 26.499 | 51.528 | 1.00 | 12.38 | A |
| ATOM | 893 | CA  | TRP | A | 123 | 50.365 | 25.390 | 50.580 | 1.00 | 10.94 | A |
| ATOM | 894 | CB  | TRP | A | 123 | 51.330 | 25.597 | 49.406 | 1.00 | 10.33 | A |
| ATOM | 895 | CG  | TRP | A | 123 | 50.761 | 26.503 | 48.337 | 1.00 | 12.83 | A |
| ATOM | 896 | CD2 | TRP | A | 123 | 49.900 | 26.108 | 47.261 | 1.00 | 10.58 | A |
| ATOM | 897 | CE2 | TRP | A | 123 | 49.568 | 27.279 | 46.533 | 1.00 | 12.26 | A |
| ATOM | 898 | CE3 | TRP | A | 123 | 49.381 | 24.884 | 46.841 | 1.00 | 12.52 | A |
| ATOM | 899 | CD1 | TRP | A | 123 | 50.916 | 27.862 | 48.227 | 1.00 | 15.24 | A |
| ATOM | 900 | NE1 | TRP | A | 123 | 50.198 | 28.334 | 47.140 | 1.00 | 12.70 | A |
| ATOM | 901 | CZ2 | TRP | A | 123 | 48.732 | 27.256 | 45.403 | 1.00 | 10.92 | A |
| ATOM | 902 | CZ3 | TRP | A | 123 | 48.547 | 24.863 | 45.710 | 1.00 | 16.36 | A |
| ATOM | 903 | CH2 | TRP | A | 123 | 48.237 | 26.043 | 45.012 | 1.00 | 9.72  | A |
| ATOM | 904 | C   | TRP | A | 123 | 50.661 | 24.045 | 51.213 | 1.00 | 13.55 | A |
| ATOM | 905 | O   | TRP | A | 123 | 50.284 | 23.006 | 50.676 | 1.00 | 13.98 | A |
| ATOM | 906 | N   | SER | A | 124 | 51.346 | 24.054 | 52.349 | 1.00 | 13.10 | A |
| ATOM | 907 | CA  | SER | A | 124 | 51.654 | 22.801 | 53.010 | 1.00 | 11.36 | A |

FIGURE 5 (suite)

|      |     |     |     |   |     |        |        |        |      |       |   |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 908 | CB  | SER | A | 124 | 52.670 | 23.038 | 54.135 | 1.00 | 11.89 | A |
| ATOM | 909 | OG  | SER | A | 124 | 52.130 | 23.884 | 55.132 | 1.00 | 14.19 | A |
| ATOM | 910 | C   | SER | A | 124 | 50.361 | 22.161 | 53.564 | 1.00 | 17.25 | A |
| ATOM | 911 | O   | SER | A | 124 | 50.354 | 20.974 | 53.924 | 1.00 | 13.81 | A |
| ATOM | 912 | N   | GLY | A | 125 | 49.273 | 22.937 | 53.617 | 1.00 | 13.73 | A |
| ATOM | 913 | CA  | GLY | A | 125 | 47.999 | 22.416 | 54.117 | 1.00 | 13.26 | A |
| ATOM | 914 | C   | GLY | A | 125 | 47.216 | 21.569 | 53.101 | 1.00 | 19.05 | A |
| ATOM | 915 | O   | GLY | A | 125 | 46.116 | 21.066 | 53.404 | 1.00 | 15.82 | A |
| ATOM | 916 | N   | ILE | A | 126 | 47.759 | 21.413 | 51.892 | 1.00 | 11.57 | A |
| ATOM | 917 | CA  | ILE | A | 126 | 47.111 | 20.590 | 50.866 | 1.00 | 13.57 | A |
| ATOM | 918 | CB  | ILE | A | 126 | 47.116 | 21.338 | 49.499 | 1.00 | 10.65 | A |
| ATOM | 919 | CG2 | ILE | A | 126 | 46.584 | 20.440 | 48.369 | 1.00 | 10.73 | A |
| ATOM | 920 | CG1 | ILE | A | 126 | 46.244 | 22.598 | 49.639 | 1.00 | 14.04 | A |
| ATOM | 921 | CD1 | ILE | A | 126 | 46.355 | 23.571 | 48.474 | 1.00 | 21.47 | A |
| ATOM | 922 | C   | ILE | A | 126 | 47.886 | 19.270 | 50.794 | 1.00 | 14.42 | A |
| ATOM | 923 | O   | ILE | A | 126 | 49.012 | 19.228 | 50.299 | 1.00 | 12.48 | A |
| ATOM | 924 | N   | THR | A | 127 | 47.287 | 18.199 | 51.310 | 1.00 | 14.33 | A |
| ATOM | 925 | CA  | THR | A | 127 | 47.974 | 16.918 | 51.341 | 1.00 | 15.70 | A |
| ATOM | 926 | CB  | THR | A | 127 | 47.144 | 15.848 | 52.079 | 1.00 | 20.78 | A |
| ATOM | 927 | OG1 | THR | A | 127 | 45.978 | 15.519 | 51.309 | 1.00 | 21.71 | A |
| ATOM | 928 | CG2 | THR | A | 127 | 46.719 | 16.379 | 53.462 | 1.00 | 19.06 | A |
| ATOM | 929 | C   | THR | A | 127 | 48.389 | 16.389 | 49.978 | 1.00 | 15.85 | A |
| ATOM | 930 | O   | THR | A | 127 | 47.628 | 16.442 | 49.011 | 1.00 | 15.48 | A |
| ATOM | 931 | N   | GLY | A | 128 | 49.627 | 15.907 | 49.925 | 1.00 | 11.25 | A |
| ATOM | 932 | CA  | GLY | A | 128 | 50.202 | 15.348 | 48.719 | 1.00 | 13.92 | A |
| ATOM | 933 | C   | GLY | A | 128 | 50.726 | 16.299 | 47.655 | 1.00 | 15.93 | A |
| ATOM | 934 | O   | GLY | A | 128 | 51.360 | 15.837 | 46.718 | 1.00 | 18.28 | A |
| ATOM | 935 | N   | ALA | A | 129 | 50.491 | 17.610 | 47.788 | 1.00 | 13.36 | A |
| ATOM | 936 | CA  | ALA | A | 129 | 50.929 | 18.558 | 46.765 | 1.00 | 14.53 | A |
| ATOM | 937 | CB  | ALA | A | 129 | 50.138 | 19.873 | 46.886 | 1.00 | 13.51 | A |
| ATOM | 938 | C   | ALA | A | 129 | 52.428 | 18.856 | 46.777 | 1.00 | 20.08 | A |
| ATOM | 939 | O   | ALA | A | 129 | 52.954 | 19.427 | 45.811 | 1.00 | 13.92 | A |
| ATOM | 940 | N   | GLY | A | 130 | 53.110 | 18.489 | 47.863 | 1.00 | 15.72 | A |
| ATOM | 941 | CA  | GLY | A | 130 | 54.552 | 18.715 | 47.931 | 1.00 | 18.22 | A |
| ATOM | 942 | C   | GLY | A | 130 | 54.937 | 20.167 | 47.720 | 1.00 | 17.01 | A |
| ATOM | 943 | O   | GLY | A | 130 | 55.944 | 20.485 | 47.088 | 1.00 | 16.95 | A |
| ATOM | 944 | N   | ARG | A | 131 | 54.130 | 21.059 | 48.274 | 1.00 | 14.88 | A |
| ATOM | 945 | CA  | ARG | A | 131 | 54.361 | 22.500 | 48.142 | 1.00 | 14.67 | A |
| ATOM | 946 | CB  | ARG | A | 131 | 53.312 | 23.102 | 47.190 | 1.00 | 10.65 | A |
| ATOM | 947 | CG  | ARG | A | 131 | 53.506 | 22.713 | 45.730 | 1.00 | 14.78 | A |
| ATOM | 948 | CD  | ARG | A | 131 | 52.234 | 22.985 | 44.895 | 1.00 | 13.27 | A |
| ATOM | 949 | NE  | ARG | A | 131 | 52.479 | 22.959 | 43.441 | 1.00 | 13.40 | A |
| ATOM | 950 | CZ  | ARG | A | 131 | 52.670 | 21.873 | 42.695 | 1.00 | 12.12 | A |
| ATOM | 951 | NH1 | ARG | A | 131 | 52.880 | 22.010 | 41.383 | 1.00 | 12.83 | A |
| ATOM | 952 | NH2 | ARG | A | 131 | 52.656 | 20.660 | 43.233 | 1.00 | 13.76 | A |
| ATOM | 953 | C   | ARG | A | 131 | 54.217 | 23.171 | 49.502 | 1.00 | 14.12 | A |
| ATOM | 954 | O   | ARG | A | 131 | 53.451 | 22.703 | 50.329 | 1.00 | 15.12 | A |
| ATOM | 955 | N   | SER | A | 132 | 54.948 | 24.258 | 49.730 | 1.00 | 12.39 | A |
| ATOM | 956 | CA  | SER | A | 132 | 54.830 | 24.987 | 50.990 | 1.00 | 15.94 | A |
| ATOM | 957 | CB  | SER | A | 132 | 55.817 | 24.450 | 52.046 | 1.00 | 22.25 | A |
| ATOM | 958 | OG  | SER | A | 132 | 57.143 | 24.690 | 51.644 | 1.00 | 25.99 | A |
| ATOM | 959 | C   | SER | A | 132 | 55.070 | 26.468 | 50.735 | 1.00 | 12.92 | A |
| ATOM | 960 | O   | SER | A | 132 | 55.695 | 26.857 | 49.746 | 1.00 | 16.84 | A |
| ATOM | 961 | N   | GLY | A | 133 | 54.570 | 27.300 | 51.634 | 1.00 | 14.33 | A |
| ATOM | 962 | CA  | GLY | A | 133 | 54.695 | 28.734 | 51.442 | 1.00 | 14.73 | A |
| ATOM | 963 | C   | GLY | A | 133 | 53.295 | 29.318 | 51.394 | 1.00 | 14.56 | A |
| ATOM | 964 | O   | GLY | A | 133 | 52.320 | 28.589 | 51.183 | 1.00 | 12.31 | A |
| ATOM | 965 | N   | PRO | A | 134 | 53.162 | 30.633 | 51.561 | 1.00 | 15.09 | A |
| ATOM | 966 | CD  | PRO | A | 134 | 54.254 | 31.607 | 51.743 | 1.00 | 16.35 | A |
| ATOM | 967 | CA  | PRO | A | 134 | 51.854 | 31.291 | 51.548 | 1.00 | 14.55 | A |
| ATOM | 968 | CB  | PRO | A | 134 | 52.196 | 32.760 | 51.828 | 1.00 | 20.54 | A |
| ATOM | 969 | CG  | PRO | A | 134 | 53.623 | 32.900 | 51.266 | 1.00 | 21.58 | A |
| ATOM | 970 | C   | PRO | A | 134 | 50.997 | 31.143 | 50.299 | 1.00 | 16.29 | A |
| ATOM | 971 | O   | PRO | A | 134 | 51.509 | 31.105 | 49.180 | 1.00 | 12.69 | A |
| ATOM | 972 | N   | ILE | A | 135 | 49.685 | 31.057 | 50.527 | 1.00 | 13.39 | A |
| ATOM | 973 | CA  | ILE | A | 135 | 48.688 | 30.973 | 49.454 | 1.00 | 13.74 | A |
| ATOM | 974 | CB  | ILE | A | 135 | 47.523 | 30.010 | 49.801 | 1.00 | 15.95 | A |
| ATOM | 975 | CG2 | ILE | A | 135 | 46.417 | 30.115 | 48.727 | 1.00 | 13.97 | A |
| ATOM | 976 | CG1 | ILE | A | 135 | 48.032 | 28.582 | 49.918 | 1.00 | 15.73 | A |
| ATOM | 977 | CD1 | ILE | A | 135 | 46.988 | 27.607 | 50.453 | 1.00 | 15.61 | A |
| ATOM | 978 | C   | ILE | A | 135 | 48.077 | 32.366 | 49.353 | 1.00 | 13.04 | A |
| ATOM | 979 | O   | ILE | A | 135 | 47.757 | 32.983 | 50.372 | 1.00 | 15.69 | A |
| ATOM | 980 | N   | GLN | A | 136 | 47.918 | 32.872 | 48.136 | 1.00 | 11.91 | A |
| ATOM | 981 | CA  | GLN | A | 136 | 47.319 | 34.190 | 47.958 | 1.00 | 11.20 | A |
| ATOM | 982 | CB  | GLN | A | 136 | 48.317 | 35.145 | 47.306 | 1.00 | 12.71 | A |
| ATOM | 983 | CG  | GLN | A | 136 | 47.892 | 36.594 | 47.337 | 1.00 | 19.42 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 984  | CD  | GLN | A | 136 | 48.999 | 37.566 | 46.905 | 1.00 | 23.10 | A |
| ATOM | 985  | OE1 | GLN | A | 136 | 49.620 | 37.403 | 45.858 | 1.00 | 23.52 | A |
| ATOM | 986  | NE2 | GLN | A | 136 | 49.233 | 38.585 | 47.714 | 1.00 | 30.84 | A |
| ATOM | 987  | C   | GLN | A | 136 | 46.105 | 34.023 | 47.053 | 1.00 | 9.51  | A |
| ATOM | 988  | O   | GLN | A | 136 | 46.254 | 33.639 | 45.921 | 1.00 | 9.81  | A |
| ATOM | 989  | N   | VAL | A | 137 | 44.911 | 34.303 | 47.552 | 1.00 | 8.18  | A |
| ATOM | 990  | CA  | VAL | A | 137 | 43.717 | 34.161 | 46.733 | 1.00 | 4.96  | A |
| ATOM | 991  | CB  | VAL | A | 137 | 42.470 | 33.907 | 47.657 | 1.00 | 8.36  | A |
| ATOM | 992  | CG1 | VAL | A | 137 | 41.176 | 34.014 | 46.855 | 1.00 | 5.20  | A |
| ATOM | 993  | CG2 | VAL | A | 137 | 42.589 | 32.543 | 48.294 | 1.00 | 10.61 | A |
| ATOM | 994  | C   | VAL | A | 137 | 43.442 | 35.380 | 45.837 | 1.00 | 9.91  | A |
| ATOM | 995  | O   | VAL | A | 137 | 43.555 | 36.534 | 46.284 | 1.00 | 9.14  | A |
| ATOM | 996  | N   | VAL | A | 138 | 43.124 | 35.114 | 44.566 | 1.00 | 7.01  | A |
| ATOM | 997  | CA  | VAL | A | 138 | 42.735 | 36.134 | 43.600 | 1.00 | 8.67  | A |
| ATOM | 998  | CB  | VAL | A | 138 | 43.437 | 35.976 | 42.226 | 1.00 | 9.91  | A |
| ATOM | 999  | CG1 | VAL | A | 138 | 42.983 | 37.092 | 41.301 | 1.00 | 11.71 | A |
| ATOM | 1000 | CG2 | VAL | A | 138 | 44.947 | 36.068 | 42.394 | 1.00 | 18.67 | A |
| ATOM | 1001 | C   | VAL | A | 138 | 41.237 | 35.914 | 43.386 | 1.00 | 7.40  | A |
| ATOM | 1002 | O   | VAL | A | 138 | 40.791 | 34.775 | 43.196 | 1.00 | 7.75  | A |
| ATOM | 1003 | N   | TYR | A | 139 | 40.452 | 36.987 | 43.435 | 1.00 | 9.87  | A |
| ATOM | 1004 | CA  | TYR | A | 139 | 39.009 | 36.871 | 43.256 | 1.00 | 9.42  | A |
| ATOM | 1005 | CB  | TYR | A | 139 | 38.303 | 36.902 | 44.625 | 1.00 | 8.26  | A |
| ATOM | 1006 | CG  | TYR | A | 139 | 38.509 | 38.192 | 45.389 | 1.00 | 9.37  | A |
| ATOM | 1007 | CD1 | TYR | A | 139 | 37.570 | 39.211 | 45.322 | 1.00 | 8.61  | A |
| ATOM | 1008 | CE1 | TYR | A | 139 | 37.748 | 40.424 | 46.013 | 1.00 | 9.72  | A |
| ATOM | 1009 | CD2 | TYR | A | 139 | 39.659 | 38.397 | 46.177 | 1.00 | 9.71  | A |
| ATOM | 1010 | CE2 | TYR | A | 139 | 39.853 | 39.616 | 46.878 | 1.00 | 12.90 | A |
| ATOM | 1011 | CZ  | TYR | A | 139 | 38.890 | 40.623 | 46.786 | 1.00 | 15.66 | A |
| ATOM | 1012 | OH  | TYR | A | 139 | 39.045 | 41.829 | 47.459 | 1.00 | 8.23  | A |
| ATOM | 1013 | C   | TYR | A | 139 | 38.507 | 38.006 | 42.381 | 1.00 | 8.45  | A |
| ATOM | 1014 | O   | TYR | A | 139 | 39.246 | 38.947 | 42.099 | 1.00 | 8.15  | A |
| ATOM | 1015 | N   | ARG | A | 140 | 37.259 | 37.899 | 41.935 | 1.00 | 8.93  | A |
| ATOM | 1016 | CA  | ARG | A | 140 | 36.660 | 38.903 | 41.070 | 1.00 | 7.41  | A |
| ATOM | 1017 | CB  | ARG | A | 140 | 35.514 | 38.296 | 40.243 | 1.00 | 10.32 | A |
| ATOM | 1018 | CG  | ARG | A | 140 | 35.991 | 37.317 | 39.148 | 1.00 | 5.86  | A |
| ATOM | 1019 | CD  | ARG | A | 140 | 36.556 | 38.103 | 37.948 | 1.00 | 5.80  | A |
| ATOM | 1020 | NE  | ARG | A | 140 | 35.502 | 38.821 | 37.218 | 1.00 | 7.23  | A |
| ATOM | 1021 | CZ  | ARG | A | 140 | 34.659 | 38.232 | 36.376 | 1.00 | 11.87 | A |
| ATOM | 1022 | NH1 | ARG | A | 140 | 34.748 | 36.918 | 36.152 | 1.00 | 5.93  | A |
| ATOM | 1023 | NH2 | ARG | A | 140 | 33.715 | 38.952 | 35.769 | 1.00 | 8.31  | A |
| ATOM | 1024 | C   | ARG | A | 140 | 36.129 | 40.063 | 41.895 | 1.00 | 8.44  | A |
| ATOM | 1025 | O   | ARG | A | 140 | 35.327 | 39.896 | 42.832 | 1.00 | 8.91  | A |
| ATOM | 1026 | N   | ALA | A | 141 | 36.583 | 41.242 | 41.523 | 1.00 | 8.44  | A |
| ATOM | 1027 | CA  | ALA | A | 141 | 36.198 | 42.471 | 42.206 | 1.00 | 8.99  | A |
| ATOM | 1028 | CB  | ALA | A | 141 | 37.121 | 43.579 | 41.761 | 1.00 | 12.40 | A |
| ATOM | 1029 | C   | ALA | A | 141 | 34.748 | 42.895 | 41.975 | 1.00 | 11.15 | A |
| ATOM | 1030 | O   | ALA | A | 141 | 34.091 | 43.421 | 42.878 | 1.00 | 9.17  | A |
| ATOM | 1031 | N   | GLU | A | 142 | 34.258 | 42.679 | 40.765 | 1.00 | 10.41 | A |
| ATOM | 1032 | CA  | GLU | A | 142 | 32.912 | 43.110 | 40.401 | 1.00 | 11.28 | A |
| ATOM | 1033 | CB  | GLU | A | 142 | 32.944 | 43.735 | 38.995 | 1.00 | 11.17 | A |
| ATOM | 1034 | CG  | GLU | A | 142 | 32.968 | 42.720 | 37.800 | 1.00 | 16.02 | A |
| ATOM | 1035 | CD  | GLU | A | 142 | 34.319 | 41.984 | 37.551 | 1.00 | 14.71 | A |
| ATOM | 1036 | OE1 | GLU | A | 142 | 35.102 | 41.758 | 38.492 | 1.00 | 20.26 | A |
| ATOM | 1037 | OE2 | GLU | A | 142 | 34.582 | 41.608 | 36.382 | 1.00 | 15.07 | A |
| ATOM | 1038 | C   | GLU | A | 142 | 31.854 | 42.001 | 40.428 | 1.00 | 15.45 | A |
| ATOM | 1039 | O   | GLU | A | 142 | 32.160 | 40.827 | 40.689 | 1.00 | 11.17 | A |
| ATOM | 1040 | N   | VAL | A | 143 | 30.604 | 42.399 | 40.170 | 1.00 | 13.82 | A |
| ATOM | 1041 | CA  | VAL | A | 143 | 29.474 | 41.461 | 40.114 | 1.00 | 12.65 | A |
| ATOM | 1042 | CB  | VAL | A | 143 | 28.155 | 42.192 | 39.792 | 1.00 | 12.26 | A |
| ATOM | 1043 | CG1 | VAL | A | 143 | 27.052 | 41.196 | 39.668 | 1.00 | 17.81 | A |
| ATOM | 1044 | CG2 | VAL | A | 143 | 27.822 | 43.174 | 40.870 | 1.00 | 18.80 | A |
| ATOM | 1045 | C   | VAL | A | 143 | 29.770 | 40.456 | 38.996 | 1.00 | 12.06 | A |
| ATOM | 1046 | O   | VAL | A | 143 | 29.785 | 40.814 | 37.811 | 1.00 | 10.75 | A |
| ATOM | 1047 | N   | SER | A | 144 | 29.972 | 39.198 | 39.388 | 1.00 | 10.21 | A |
| ATOM | 1048 | CA  | SER | A | 144 | 30.352 | 38.119 | 38.462 | 1.00 | 6.60  | A |
| ATOM | 1049 | CB  | SER | A | 144 | 31.822 | 37.764 | 38.758 | 1.00 | 8.21  | A |
| ATOM | 1050 | OG  | SER | A | 144 | 32.188 | 36.468 | 38.328 | 1.00 | 8.64  | A |
| ATOM | 1051 | C   | SER | A | 144 | 29.499 | 36.834 | 38.512 | 1.00 | 7.57  | A |
| ATOM | 1052 | O   | SER | A | 144 | 29.166 | 36.346 | 39.601 | 1.00 | 8.05  | A |
| ATOM | 1053 | N   | GLY | A | 145 | 29.168 | 36.303 | 37.330 | 1.00 | 5.34  | A |
| ATOM | 1054 | CA  | GLY | A | 145 | 28.437 | 35.047 | 37.226 | 1.00 | 7.72  | A |
| ATOM | 1055 | C   | GLY | A | 145 | 29.335 | 33.884 | 37.638 | 1.00 | 7.84  | A |
| ATOM | 1056 | O   | GLY | A | 145 | 28.873 | 32.870 | 38.197 | 1.00 | 6.69  | A |
| ATOM | 1057 | N   | THR | A | 146 | 30.628 | 34.001 | 37.357 | 1.00 | 6.57  | A |
| ATOM | 1058 | CA  | THR | A | 146 | 31.574 | 32.953 | 37.758 | 1.00 | 6.39  | A |
| ATOM | 1059 | CB  | THR | A | 146 | 33.012 | 33.263 | 37.279 | 1.00 | 9.37  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1060 | OG1 | THR | A | 146 | 33.026 | 33.463 | 35.855 | 1.00 | 8.49  | A |
| ATOM | 1061 | CG2 | THR | A | 146 | 33.928 | 32.087 | 37.613 | 1.00 | 11.25 | A |
| ATOM | 1062 | C   | THR | A | 146 | 31.569 | 32.892 | 39.294 | 1.00 | 8.02  | A |
| ATOM | 1063 | O   | THR | A | 146 | 31.601 | 31.802 | 39.888 | 1.00 | 8.00  | A |
| ATOM | 1064 | N   | THR | A | 147 | 31.551 | 34.064 | 39.930 | 1.00 | 6.33  | A |
| ATOM | 1065 | CA  | THR | A | 147 | 31.483 | 34.131 | 41.394 | 1.00 | 8.35  | A |
| ATOM | 1066 | CB  | THR | A | 147 | 31.554 | 35.591 | 41.921 | 1.00 | 6.29  | A |
| ATOM | 1067 | OG1 | THR | A | 147 | 32.834 | 36.161 | 41.624 | 1.00 | 7.92  | A |
| ATOM | 1068 | CG2 | THR | A | 147 | 31.373 | 35.602 | 43.450 | 1.00 | 8.46  | A |
| ATOM | 1069 | C   | THR | A | 147 | 30.175 | 33.486 | 41.885 | 1.00 | 5.86  | A |
| ATOM | 1070 | O   | THR | A | 147 | 30.172 | 32.745 | 42.883 | 1.00 | 7.90  | A |
| ATOM | 1071 | N   | GLU | A | 148 | 29.059 | 33.751 | 41.198 | 1.00 | 5.81  | A |
| ATOM | 1072 | CA  | GLU | A | 148 | 27.786 | 33.131 | 41.592 | 1.00 | 5.50  | A |
| ATOM | 1073 | CB  | GLU | A | 148 | 26.644 | 33.653 | 40.710 | 1.00 | 6.06  | A |
| ATOM | 1074 | CG  | GLU | A | 148 | 25.284 | 33.004 | 41.058 | 1.00 | 10.99 | A |
| ATOM | 1075 | CD  | GLU | A | 148 | 24.076 | 33.737 | 40.457 | 1.00 | 12.04 | A |
| ATOM | 1076 | OE1 | GLU | A | 148 | 23.920 | 34.966 | 40.685 | 1.00 | 9.92  | A |
| ATOM | 1077 | OE2 | GLU | A | 148 | 23.271 | 33.078 | 39.765 | 1.00 | 13.03 | A |
| ATOM | 1078 | C   | GLU | A | 148 | 27.846 | 31.591 | 41.491 | 1.00 | 6.20  | A |
| ATOM | 1079 | O   | GLU | A | 148 | 27.419 | 30.866 | 42.408 | 1.00 | 7.44  | A |
| ATOM | 1080 | N   | LEU | A | 149 | 28.318 | 31.077 | 40.359 | 1.00 | 4.66  | A |
| ATOM | 1081 | CA  | LEU | A | 149 | 28.442 | 29.616 | 40.196 | 1.00 | 6.87  | A |
| ATOM | 1082 | CB  | LEU | A | 149 | 29.011 | 29.301 | 38.807 | 1.00 | 7.74  | A |
| ATOM | 1083 | CG  | LEU | A | 149 | 28.105 | 29.569 | 37.591 | 1.00 | 8.75  | A |
| ATOM | 1084 | CD1 | LEU | A | 149 | 28.878 | 29.218 | 36.342 | 1.00 | 10.50 | A |
| ATOM | 1085 | CD2 | LEU | A | 149 | 26.804 | 28.721 | 37.678 | 1.00 | 9.52  | A |
| ATOM | 1086 | C   | LEU | A | 149 | 29.376 | 28.980 | 41.254 | 1.00 | 7.07  | A |
| ATOM | 1087 | O   | LEU | A | 149 | 29.127 | 27.865 | 41.754 | 1.00 | 7.65  | A |
| ATOM | 1088 | N   | PHE | A | 150 | 30.473 | 29.670 | 41.568 | 1.00 | 8.71  | A |
| ATOM | 1089 | CA  | PHE | A | 150 | 31.459 | 29.183 | 42.540 | 1.00 | 7.06  | A |
| ATOM | 1090 | CB  | PHE | A | 150 | 32.752 | 30.021 | 42.427 | 1.00 | 6.97  | A |
| ATOM | 1091 | CG  | PHE | A | 150 | 33.884 | 29.551 | 43.325 | 1.00 | 9.24  | A |
| ATOM | 1092 | CD1 | PHE | A | 150 | 34.313 | 28.225 | 43.305 | 1.00 | 10.27 | A |
| ATOM | 1093 | CD2 | PHE | A | 150 | 34.557 | 30.455 | 44.138 | 1.00 | 12.03 | A |
| ATOM | 1094 | CE1 | PHE | A | 150 | 35.411 | 27.803 | 44.081 | 1.00 | 12.21 | A |
| ATOM | 1095 | CE2 | PHE | A | 150 | 35.657 | 30.050 | 44.920 | 1.00 | 11.31 | A |
| ATOM | 1096 | CZ  | PHE | A | 150 | 36.083 | 28.721 | 44.890 | 1.00 | 10.56 | A |
| ATOM | 1097 | C   | PHE | A | 150 | 30.936 | 29.217 | 43.987 | 1.00 | 7.58  | A |
| ATOM | 1098 | O   | PHE | A | 150 | 31.060 | 28.236 | 44.709 | 1.00 | 6.52  | A |
| ATOM | 1099 | N   | THR | A | 151 | 30.350 | 30.334 | 44.409 | 1.00 | 7.57  | A |
| ATOM | 1100 | CA  | THR | A | 151 | 29.836 | 30.437 | 45.770 | 1.00 | 8.97  | A |
| ATOM | 1101 | CB  | THR | A | 151 | 29.548 | 31.938 | 46.193 | 1.00 | 9.78  | A |
| ATOM | 1102 | OG1 | THR | A | 151 | 28.580 | 32.526 | 45.314 | 1.00 | 8.77  | A |
| ATOM | 1103 | CG2 | THR | A | 151 | 30.826 | 32.744 | 46.152 | 1.00 | 7.96  | A |
| ATOM | 1104 | C   | THR | A | 151 | 28.588 | 29.588 | 45.988 | 1.00 | 7.22  | A |
| ATOM | 1105 | O   | THR | A | 151 | 28.274 | 29.245 | 47.131 | 1.00 | 7.49  | A |
| ATOM | 1106 | N   | ARG | A | 152 | 27.873 | 29.229 | 44.916 | 1.00 | 5.13  | A |
| ATOM | 1107 | CA  | ARG | A | 152 | 26.715 | 28.351 | 45.099 | 1.00 | 9.17  | A |
| ATOM | 1108 | CB  | ARG | A | 152 | 25.914 | 28.189 | 43.796 | 1.00 | 9.15  | A |
| ATOM | 1109 | CG  | ARG | A | 152 | 24.606 | 27.376 | 43.974 | 1.00 | 10.79 | A |
| ATOM | 1110 | CD  | ARG | A | 152 | 23.671 | 27.529 | 42.755 | 1.00 | 17.61 | A |
| ATOM | 1111 | NE  | ARG | A | 152 | 23.071 | 28.868 | 42.641 | 1.00 | 14.93 | A |
| ATOM | 1112 | CZ  | ARG | A | 152 | 23.188 | 29.662 | 41.577 | 1.00 | 16.78 | A |
| ATOM | 1113 | NH1 | ARG | A | 152 | 22.605 | 30.860 | 41.565 | 1.00 | 11.71 | A |
| ATOM | 1114 | NH2 | ARG | A | 152 | 23.885 | 29.265 | 40.518 | 1.00 | 11.02 | A |
| ATOM | 1115 | C   | ARG | A | 152 | 27.274 | 27.007 | 45.557 | 1.00 | 7.79  | A |
| ATOM | 1116 | O   | ARG | A | 152 | 26.671 | 26.313 | 46.389 | 1.00 | 5.08  | A |
| ATOM | 1117 | N   | PHE | A | 153 | 28.436 | 26.639 | 45.017 | 1.00 | 6.70  | A |
| ATOM | 1118 | CA  | PHE | A | 153 | 29.101 | 25.395 | 45.413 | 1.00 | 9.70  | A |
| ATOM | 1119 | CB  | PHE | A | 153 | 30.280 | 25.059 | 44.478 | 1.00 | 7.27  | A |
| ATOM | 1120 | CG  | PHE | A | 153 | 30.974 | 23.747 | 44.812 | 1.00 | 6.93  | A |
| ATOM | 1121 | CD1 | PHE | A | 153 | 30.451 | 22.532 | 44.389 | 1.00 | 9.41  | A |
| ATOM | 1122 | CD2 | PHE | A | 153 | 32.134 | 23.738 | 45.592 | 1.00 | 9.61  | A |
| ATOM | 1123 | CE1 | PHE | A | 153 | 31.069 | 21.315 | 44.747 | 1.00 | 11.43 | A |
| ATOM | 1124 | CE2 | PHE | A | 153 | 32.764 | 22.534 | 45.959 | 1.00 | 13.90 | A |
| ATOM | 1125 | CZ  | PHE | A | 153 | 32.229 | 21.323 | 45.537 | 1.00 | 11.19 | A |
| ATOM | 1126 | C   | PHE | A | 153 | 29.640 | 25.503 | 46.842 | 1.00 | 8.50  | A |
| ATOM | 1127 | O   | PHE | A | 153 | 29.455 | 24.586 | 47.638 | 1.00 | 8.41  | A |
| ATOM | 1128 | N   | LEU | A | 154 | 30.320 | 26.599 | 47.167 | 1.00 | 6.84  | A |
| ATOM | 1129 | CA  | LEU | A | 154 | 30.877 | 26.752 | 48.521 | 1.00 | 6.20  | A |
| ATOM | 1130 | CB  | LEU | A | 154 | 31.672 | 28.060 | 48.657 | 1.00 | 6.23  | A |
| ATOM | 1131 | CG  | LEU | A | 154 | 32.876 | 28.250 | 47.720 | 1.00 | 6.30  | A |
| ATOM | 1132 | CD1 | LEU | A | 154 | 33.543 | 29.583 | 48.020 | 1.00 | 9.48  | A |
| ATOM | 1133 | CD2 | LEU | A | 154 | 33.893 | 27.117 | 47.886 | 1.00 | 6.15  | A |
| ATOM | 1134 | C   | LEU | A | 154 | 29.762 | 26.737 | 49.564 | 1.00 | 6.13  | A |
| ATOM | 1135 | O   | LEU | A | 154 | 29.912 | 26.170 | 50.641 | 1.00 | 9.16  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1136 | N   | ASN | A | 155 | 28.652 | 27.376 | 49.233 | 1.00 | 5.19  | A |
| ATOM | 1137 | CA  | ASN | A | 155 | 27.493 | 27.430 | 50.116 | 1.00 | 6.32  | A |
| ATOM | 1138 | CB  | ASN | A | 155 | 26.406 | 28.314 | 49.486 | 1.00 | 11.33 | A |
| ATOM | 1139 | CG  | ASN | A | 155 | 25.093 | 28.294 | 50.274 | 1.00 | 14.59 | A |
| ATOM | 1140 | OD1 | ASN | A | 155 | 24.149 | 27.596 | 49.906 | 1.00 | 9.21  | A |
| ATOM | 1141 | ND2 | ASN | A | 155 | 25.034 | 29.062 | 51.361 | 1.00 | 8.23  | A |
| ATOM | 1142 | C   | ASN | A | 155 | 26.929 | 26.042 | 50.363 | 1.00 | 8.76  | A |
| ATOM | 1143 | O   | ASN | A | 155 | 26.465 | 25.712 | 51.465 | 1.00 | 8.00  | A |
| ATOM | 1144 | N   | ALA | A | 156 | 26.965 | 25.203 | 49.336 | 1.00 | 8.80  | A |
| ATOM | 1145 | CA  | ALA | A | 156 | 26.418 | 23.867 | 49.493 | 1.00 | 7.63  | A |
| ATOM | 1146 | CB  | ALA | A | 156 | 26.068 | 23.300 | 48.119 | 1.00 | 8.06  | A |
| ATOM | 1147 | C   | ALA | A | 156 | 27.336 | 22.882 | 50.222 | 1.00 | 12.23 | A |
| ATOM | 1148 | O   | ALA | A | 156 | 26.854 | 22.037 | 50.994 | 1.00 | 9.62  | A |
| ATOM | 1149 | N   | LYS | A | 157 | 28.646 | 23.029 | 50.015 | 1.00 | 9.93  | A |
| ATOM | 1150 | CA  | LYS | A | 157 | 29.623 | 22.064 | 50.537 | 1.00 | 10.69 | A |
| ATOM | 1151 | CB  | LYS | A | 157 | 30.437 | 21.527 | 49.352 | 1.00 | 14.97 | A |
| ATOM | 1152 | CG  | LYS | A | 157 | 29.604 | 20.877 | 48.227 | 1.00 | 13.56 | A |
| ATOM | 1153 | CD  | LYS | A | 157 | 28.855 | 19.640 | 48.729 | 1.00 | 16.77 | A |
| ATOM | 1154 | CE  | LYS | A | 157 | 28.357 | 18.784 | 47.575 | 1.00 | 22.67 | A |
| ATOM | 1155 | NZ  | LYS | A | 157 | 27.652 | 17.546 | 48.069 | 1.00 | 21.73 | A |
| ATOM | 1156 | C   | LYS | A | 157 | 30.611 | 22.438 | 51.638 | 1.00 | 8.73  | A |
| ATOM | 1157 | O   | LYS | A | 157 | 31.215 | 21.552 | 52.245 | 1.00 | 11.63 | A |
| ATOM | 1158 | N   | CYS | A | 158 | 30.821 | 23.725 | 51.876 | 1.00 | 8.12  | A |
| ATOM | 1159 | CA  | CYS | A | 158 | 31.759 | 24.132 | 52.916 | 1.00 | 8.20  | A |
| ATOM | 1160 | C   | CYS | A | 158 | 30.974 | 24.252 | 54.207 | 1.00 | 9.14  | A |
| ATOM | 1161 | O   | CYS | A | 158 | 30.648 | 25.349 | 54.661 | 1.00 | 10.53 | A |
| ATOM | 1162 | CB  | CYS | A | 158 | 32.390 | 25.464 | 52.537 | 1.00 | 10.13 | A |
| ATOM | 1163 | SG  | CYS | A | 158 | 33.331 | 25.358 | 50.982 | 1.00 | 11.82 | A |
| ATOM | 1164 | N   | THR | A | 159 | 30.699 | 23.108 | 54.822 | 1.00 | 8.92  | A |
| ATOM | 1165 | CA  | THR | A | 159 | 29.856 | 23.091 | 56.017 | 1.00 | 6.75  | A |
| ATOM | 1166 | CB  | THR | A | 159 | 28.850 | 21.933 | 55.903 | 1.00 | 10.13 | A |
| ATOM | 1167 | OG1 | THR | A | 159 | 29.551 | 20.690 | 55.987 | 1.00 | 12.88 | A |
| ATOM | 1168 | CG2 | THR | A | 159 | 28.146 | 21.989 | 54.527 | 1.00 | 14.84 | A |
| ATOM | 1169 | C   | THR | A | 159 | 30.545 | 23.021 | 57.361 | 1.00 | 8.62  | A |
| ATOM | 1170 | O   | THR | A | 159 | 29.878 | 22.956 | 58.398 | 1.00 | 7.39  | A |
| ATOM | 1171 | N   | THR | A | 160 | 31.875 | 23.038 | 57.358 | 1.00 | 8.39  | A |
| ATOM | 1172 | CA  | THR | A | 160 | 32.603 | 22.980 | 58.612 | 1.00 | 9.53  | A |
| ATOM | 1173 | CB  | THR | A | 160 | 33.194 | 21.558 | 58.889 | 1.00 | 8.99  | A |
| ATOM | 1174 | OG1 | THR | A | 160 | 34.011 | 21.140 | 57.788 | 1.00 | 12.55 | A |
| ATOM | 1175 | CG2 | THR | A | 160 | 32.083 | 20.559 | 59.114 | 1.00 | 11.60 | A |
| ATOM | 1176 | C   | THR | A | 160 | 33.727 | 24.010 | 58.712 | 1.00 | 10.20 | A |
| ATOM | 1177 | O   | THR | A | 160 | 34.774 | 23.739 | 59.314 | 1.00 | 8.76  | A |
| ATOM | 1178 | N   | GLN | A | 161 | 33.523 | 25.189 | 58.121 | 1.00 | 8.66  | A |
| ATOM | 1179 | CA  | GLN | A | 161 | 34.525 | 26.260 | 58.254 | 1.00 | 9.46  | A |
| ATOM | 1180 | CB  | GLN | A | 161 | 34.564 | 27.121 | 56.989 | 1.00 | 9.58  | A |
| ATOM | 1181 | CG  | GLN | A | 161 | 34.956 | 26.309 | 55.742 | 1.00 | 7.83  | A |
| ATOM | 1182 | CD  | GLN | A | 161 | 36.305 | 25.608 | 55.936 | 1.00 | 10.81 | A |
| ATOM | 1183 | OE1 | GLN | A | 161 | 36.429 | 24.396 | 55.758 | 1.00 | 12.80 | A |
| ATOM | 1184 | NE2 | GLN | A | 161 | 37.306 | 26.374 | 56.313 | 1.00 | 10.64 | A |
| ATOM | 1185 | C   | GLN | A | 161 | 34.058 | 27.096 | 59.449 | 1.00 | 8.71  | A |
| ATOM | 1186 | O   | GLN | A | 161 | 32.979 | 26.866 | 59.960 | 1.00 | 8.58  | A |
| ATOM | 1187 | N   | PRO | A | 162 | 34.870 | 28.047 | 59.928 | 1.00 | 11.51 | A |
| ATOM | 1188 | CD  | PRO | A | 162 | 36.316 | 28.193 | 59.693 | 1.00 | 10.65 | A |
| ATOM | 1189 | CA  | PRO | A | 162 | 34.433 | 28.869 | 61.071 | 1.00 | 9.23  | A |
| ATOM | 1190 | CB  | PRO | A | 162 | 35.631 | 29.780 | 61.326 | 1.00 | 11.89 | A |
| ATOM | 1191 | CG  | PRO | A | 162 | 36.786 | 28.884 | 60.979 | 1.00 | 14.39 | A |
| ATOM | 1192 | C   | PRO | A | 162 | 33.171 | 29.660 | 60.727 | 1.00 | 10.67 | A |
| ATOM | 1193 | O   | PRO | A | 162 | 32.280 | 29.838 | 61.567 | 1.00 | 12.32 | A |
| ATOM | 1194 | N   | GLY | A | 163 | 33.112 | 30.158 | 59.492 | 1.00 | 8.94  | A |
| ATOM | 1195 | CA  | GLY | A | 163 | 31.943 | 30.903 | 59.040 | 1.00 | 11.83 | A |
| ATOM | 1196 | C   | GLY | A | 163 | 31.307 | 30.149 | 57.883 | 1.00 | 11.53 | A |
| ATOM | 1197 | O   | GLY | A | 163 | 31.687 | 28.989 | 57.628 | 1.00 | 9.27  | A |
| ATOM | 1198 | N   | THR | A | 164 | 30.359 | 30.781 | 57.178 | 1.00 | 7.79  | A |
| ATOM | 1199 | CA  | THR | A | 164 | 29.698 | 30.140 | 56.039 | 1.00 | 10.06 | A |
| ATOM | 1200 | CB  | THR | A | 164 | 28.213 | 29.775 | 56.347 | 1.00 | 9.77  | A |
| ATOM | 1201 | OG1 | THR | A | 164 | 27.565 | 30.914 | 56.934 | 1.00 | 12.97 | A |
| ATOM | 1202 | CG2 | THR | A | 164 | 28.119 | 28.585 | 57.328 | 1.00 | 7.94  | A |
| ATOM | 1203 | C   | THR | A | 164 | 29.696 | 31.081 | 54.837 | 1.00 | 10.41 | A |
| ATOM | 1204 | O   | THR | A | 164 | 29.786 | 32.301 | 55.001 | 1.00 | 7.96  | A |
| ATOM | 1205 | N   | PHE | A | 165 | 29.571 | 30.507 | 53.637 | 1.00 | 7.32  | A |
| ATOM | 1206 | CA  | PHE | A | 165 | 29.551 | 31.275 | 52.395 | 1.00 | 9.34  | A |
| ATOM | 1207 | CB  | PHE | A | 165 | 30.321 | 30.541 | 51.299 | 1.00 | 8.51  | A |
| ATOM | 1208 | CG  | PHE | A | 165 | 31.799 | 30.451 | 51.539 | 1.00 | 7.69  | A |
| ATOM | 1209 | CD1 | PHE | A | 165 | 32.659 | 31.455 | 51.096 | 1.00 | 8.05  | A |
| ATOM | 1210 | CD2 | PHE | A | 165 | 32.338 | 29.338 | 52.181 | 1.00 | 10.52 | A |
| ATOM | 1211 | CE1 | PHE | A | 165 | 34.062 | 31.349 | 51.288 | 1.00 | 6.48  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |        |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|---|
| ATOM | 1212 | CE2 | PHE | A | 165 | 33.720 | 29.214 | 52.385 | 1.00 | 6.44   | A |
| ATOM | 1213 | CZ  | PHE | A | 165 | 34.591 | 30.221 | 51.935 | 1.00 | 7.86   | A |
| ATOM | 1214 | C   | PHE | A | 165 | 28.135 | 31.467 | 51.854 | 1.00 | 10.39  | A |
| ATOM | 1215 | O   | PHE | A | 165 | 27.428 | 30.485 | 51.648 | 1.00 | 11.83  | A |
| ATOM | 1216 | N   | ALA | A | 166 | 27.738 | 32.712 | 51.601 | 1.00 | 8.80   | A |
| ATOM | 1217 | CA  | ALA | A | 166 | 26.424 | 33.000 | 51.006 | 1.00 | 10.97  | A |
| ATOM | 1218 | CB  | ALA | A | 166 | 25.942 | 34.397 | 51.423 | 1.00 | 10.57  | A |
| ATOM | 1219 | C   | ALA | A | 166 | 26.593 | 32.960 | 49.483 | 1.00 | 10.58  | A |
| ATOM | 1220 | O   | ALA | A | 166 | 27.694 | 33.182 | 48.968 | 1.00 | 7.60   | A |
| ATOM | 1221 | N   | VAL | A | 167 | 25.516 | 32.668 | 49.766 | 1.00 | 9.26   | A |
| ATOM | 1222 | CA  | VAL | A | 167 | 25.572 | 32.658 | 47.303 | 1.00 | 7.71   | A |
| ATOM | 1223 | CB  | VAL | A | 167 | 24.384 | 31.924 | 46.686 | 1.00 | 7.77   | A |
| ATOM | 1224 | CG1 | VAL | A | 167 | 24.546 | 31.870 | 45.159 | 1.00 | 8.04   | A |
| ATOM | 1225 | CG2 | VAL | A | 167 | 24.283 | 30.511 | 47.265 | 1.00 | 10.61  | A |
| ATOM | 1226 | C   | VAL | A | 167 | 25.473 | 34.123 | 46.875 | 1.00 | 8.91   | A |
| ATOM | 1227 | O   | VAL | A | 167 | 24.523 | 34.816 | 47.244 | 1.00 | 7.79   | A |
| ATOM | 1228 | N   | THR | A | 168 | 26.408 | 34.580 | 46.048 | 1.00 | 8.13   | A |
| ATOM | 1229 | CA  | THR | A | 168 | 26.411 | 35.974 | 45.653 | 1.00 | 6.66   | A |
| ATOM | 1230 | CB  | THR | A | 168 | 27.060 | 36.810 | 46.769 | 1.00 | 13.46  | A |
| ATOM | 1231 | OG1 | THR | A | 168 | 27.129 | 38.188 | 46.370 | 1.00 | 12.35  | A |
| ATOM | 1232 | CG2 | THR | A | 168 | 28.478 | 36.311 | 47.040 | 1.00 | 12.28  | A |
| ATOM | 1233 | C   | THR | A | 168 | 27.228 | 36.178 | 44.375 | 1.00 | 11.69  | A |
| ATOM | 1234 | O   | THR | A | 168 | 27.960 | 35.282 | 43.947 | 1.00 | 11.22  | A |
| ATOM | 1235 | N   | THR | A | 169 | 27.106 | 37.352 | 43.770 | 1.00 | 9.36   | A |
| ATOM | 1236 | CA  | THR | A | 169 | 27.888 | 37.641 | 42.580 | 1.00 | 5.90   | A |
| ATOM | 1237 | CB  | THR | A | 169 | 27.074 | 38.484 | 41.555 | 1.00 | 11.79  | A |
| ATOM | 1238 | OG1 | THR | A | 169 | 26.724 | 39.739 | 42.159 | 1.00 | 9.77   | A |
| ATOM | 1239 | CG2 | THR | A | 169 | 25.811 | 37.747 | 41.128 | 1.00 | 12.13  | A |
| ATOM | 1240 | C   | THR | A | 169 | 29.156 | 38.450 | 42.953 | 1.00 | 9.03   | A |
| ATOM | 1241 | O   | THR | A | 169 | 30.000 | 38.712 | 42.099 | 1.00 | 8.64   | A |
| ATOM | 1242 | N   | VAL | A | 170 | 29.279 | 38.848 | 44.224 | 1.00 | 11.21  | A |
| ATOM | 1243 | CA  | VAL | A | 170 | 30.430 | 39.641 | 44.680 | 1.00 | 11.07  | A |
| ATOM | 1244 | CB  | VAL | A | 170 | 29.944 | 41.003 | 45.248 | 1.00 | 8.64   | A |
| ATOM | 1245 | CG1 | VAL | A | 170 | 29.433 | 41.863 | 44.106 | 1.00 | 8.12   | A |
| ATOM | 1246 | CG2 | VAL | A | 170 | 28.802 | 40.805 | 46.208 | 1.00 | 14.20  | A |
| ATOM | 1247 | C   | VAL | A | 170 | 31.158 | 38.830 | 45.741 | 1.00 | 10.94  | A |
| ATOM | 1248 | O   | VAL | A | 170 | 30.694 | 38.747 | 46.859 | 1.00 | 11.12  | A |
| ATOM | 1249 | N   | PHE | A | 171 | 32.305 | 38.247 | 45.386 | 1.00 | 11.66  | A |
| ATOM | 1250 | CA  | PHE | A | 171 | 33.003 | 37.367 | 46.312 | 1.00 | 9.52   | A |
| ATOM | 1251 | CB  | PHE | A | 171 | 34.279 | 36.775 | 45.677 | 1.00 | 8.67   | A |
| ATOM | 1252 | CG  | PHE | A | 171 | 34.940 | 35.686 | 46.519 | 1.00 | 10.69  | A |
| ATOM | 1253 | CD1 | PHE | A | 171 | 36.009 | 35.978 | 47.358 | 1.00 | 9.84   | A |
| ATOM | 1254 | CD2 | PHE | A | 171 | 34.457 | 34.377 | 46.502 | 1.00 | 14.44  | A |
| ATOM | 1255 | CE1 | PHE | A | 171 | 36.593 | 34.986 | 48.184 | 1.00 | 8.85   | A |
| ATOM | 1256 | CE2 | PHE | A | 171 | 35.024 | 33.377 | 47.311 | 1.00 | 12.76  | A |
| ATOM | 1257 | CZ  | PHE | A | 171 | 36.096 | 33.686 | 48.158 | 1.00 | 12..60 | A |
| ATOM | 1258 | C   | PHE | A | 171 | 33.353 | 37.977 | 47.661 | 1.00 | 12.55  | A |
| ATOM | 1259 | O   | PHE | A | 171 | 33.292 | 37.294 | 48.679 | 1.00 | 7.64   | A |
| ATOM | 1260 | N   | ALA | A | 172 | 33.704 | 39.257 | 47.677 | 1.00 | 6.57   | A |
| ATOM | 1261 | CA  | ALA | A | 172 | 34.088 | 39.865 | 48.946 | 1.00 | 9.02   | A |
| ATOM | 1262 | CB  | ALA | A | 172 | 34.655 | 41.279 | 48.721 | 1.00 | 9.26   | A |
| ATOM | 1263 | C   | ALA | A | 172 | 32.948 | 39.885 | 49.957 | 1.00 | 11.22  | A |
| ATOM | 1264 | O   | ALA | A | 172 | 33.188 | 40.071 | 51.155 | 1.00 | 10.96  | A |
| ATOM | 1265 | N   | ASN | A | 173 | 31.714 | 39.677 | 49.493 | 1.00 | 8.23   | A |
| ATOM | 1266 | CA  | ASN | A | 173 | 30.563 | 39.651 | 50.409 | 1.00 | 10.55  | A |
| ATOM | 1267 | CB  | ASN | A | 173 | 29.361 | 40.396 | 49.822 | 1.00 | 11.87  | A |
| ATOM | 1268 | CG  | ASN | A | 173 | 29.628 | 41.862 | 49.606 | 1.00 | 13.88  | A |
| ATOM | 1269 | OD1 | ASN | A | 173 | 30.289 | 42.512 | 50.412 | 1.00 | 13.36  | A |
| ATOM | 1270 | ND2 | ASN | A | 173 | 29.098 | 42.398 | 48.515 | 1.00 | 16.29  | A |
| ATOM | 1271 | C   | ASN | A | 173 | 30.062 | 38.245 | 50.759 | 1.00 | 13.21  | A |
| ATOM | 1272 | O   | ASN | A | 173 | 29.077 | 38.109 | 51.498 | 1.00 | 10.89  | A |
| ATOM | 1273 | N   | SER | A | 174 | 30.716 | 37.212 | 50.238 | 1.00 | 7.67   | A |
| ATOM | 1274 | CA  | SER | A | 174 | 30.250 | 35.859 | 50.468 | 1.00 | 9.24   | A |
| ATOM | 1275 | CB  | SER | A | 174 | 30.869 | 34.905 | 49.429 | 1.00 | 9.01   | A |
| ATOM | 1276 | OG  | SER | A | 174 | 30.359 | 33.580 | 49.598 | 1.00 | 8.15   | A |
| ATOM | 1277 | C   | SER | A | 174 | 30.440 | 35.250 | 51.863 | 1.00 | 7.73   | A |
| ATOM | 1278 | O   | SER | A | 174 | 29.480 | 34.822 | 52.506 | 1.00 | 8.54   | A |
| ATOM | 1279 | N   | TYR | A | 175 | 31.684 | 35.160 | 52.303 | 1.00 | 6.67   | A |
| ATOM | 1280 | CA  | TYR | A | 175 | 31.978 | 34.535 | 53.599 | 1.00 | 6.35   | A |
| ATOM | 1281 | CB  | TYR | A | 175 | 33.493 | 34.371 | 53.735 | 1.00 | 7.83   | A |
| ATOM | 1282 | CG  | TYR | A | 175 | 33.928 | 33.429 | 54.847 | 1.00 | 6.19   | A |
| ATOM | 1283 | CD1 | TYR | A | 175 | 34.845 | 33.842 | 55.825 | 1.00 | 9.13   | A |
| ATOM | 1284 | CE1 | TYR | A | 175 | 35.315 | 32.938 | 56.811 | 1.00 | 7.78   | A |
| ATOM | 1285 | CD2 | TYR | A | 175 | 33.481 | 32.102 | 54.879 | 1.00 | 6.63   | A |
| ATOM | 1286 | CE2 | TYR | A | 175 | 33.939 | 31.206 | 55.856 | 1.00 | 9.07   | A |
| ATOM | 1287 | CZ  | TYR | A | 175 | 34.859 | 31.633 | 56.812 | 1.00 | 11.83  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1288 | OH  | TYR | A | 175 | 35.348 | 30.731 | 57.746 | 1.00 | 8.85  | A |
| ATOM | 1289 | C   | TYR | A | 175 | 31.424 | 35.365 | 54.761 | 1.00 | 12.71 | A |
| ATOM | 1290 | O   | TYR | A | 175 | 31.649 | 36.556 | 54.806 | 1.00 | 7.92  | A |
| ATOM | 1291 | N   | SER | A | 176 | 30.695 | 34.727 | 55.683 | 1.00 | 9.13  | A |
| ATOM | 1292 | CA  | SER | A | 176 | 30.104 | 35.431 | 56.828 | 1.00 | 9.94  | A |
| ATOM | 1293 | CB  | SER | A | 176 | 29.372 | 34.433 | 57.737 | 1.00 | 11.72 | A |
| ATOM | 1294 | OG  | SER | A | 176 | 30.248 | 33.426 | 58.245 | 1.00 | 9.80  | A |
| ATOM | 1295 | C   | SER | A | 176 | 31.092 | 36.247 | 57.659 | 1.00 | 11.68 | A |
| ATOM | 1296 | O   | SER | A | 176 | 30.737 | 37.302 | 58.184 | 1.00 | 12.94 | A |
| ATOM | 1297 | N   | LEU | A | 177 | 32.332 | 35.787 | 57.788 | 1.00 | 10.90 | A |
| ATOM | 1298 | CA  | LEU | A | 177 | 33.303 | 36.559 | 58.561 | 1.00 | 12.59 | A |
| ATOM | 1299 | CB  | LEU | A | 177 | 34.231 | 35.613 | 59.349 | 1.00 | 14.55 | A |
| ATOM | 1300 | CG  | LEU | A | 177 | 33.537 | 34.649 | 60.324 | 1.00 | 15.21 | A |
| ATOM | 1301 | CD1 | LEU | A | 177 | 34.579 | 33.649 | 60.872 | 1.00 | 18.41 | A |
| ATOM | 1302 | CD2 | LEU | A | 177 | 32.856 | 35.452 | 61.476 | 1.00 | 11.73 | A |
| ATOM | 1303 | C   | LEU | A | 177 | 34.139 | 37.522 | 57.692 | 1.00 | 13.68 | A |
| ATOM | 1304 | O   | LEU | A | 177 | 35.126 | 38.104 | 58.163 | 1.00 | 12.71 | A |
| ATOM | 1305 | N   | GLY | A | 178 | 33.754 | 37.680 | 56.434 | 1.00 | 9.18  | A |
| ATOM | 1306 | CA  | GLY | A | 178 | 34.475 | 38.585 | 55.541 | 1.00 | 12.34 | A |
| ATOM | 1307 | C   | GLY | A | 178 | 35.803 | 38.098 | 54.975 | 1.00 | 12.74 | A |
| ATOM | 1308 | O   | GLY | A | 178 | 36.205 | 36.939 | 55.208 | 1.00 | 13.97 | A |
| ATOM | 1309 | N   | LEU | A | 179 | 36.492 | 38.974 | 54.224 | 1.00 | 9.84  | A |
| ATOM | 1310 | CA  | LEU | A | 179 | 37.787 | 38.610 | 53.621 | 1.00 | 10.63 | A |
| ATOM | 1311 | CB  | LEU | A | 179 | 38.078 | 39.437 | 52.350 | 1.00 | 11.33 | A |
| ATOM | 1312 | CG  | LEU | A | 179 | 37.189 | 39.202 | 51.120 | 1.00 | 10.67 | A |
| ATOM | 1313 | CD1 | LEU | A | 179 | 37.729 | 40.017 | 49.934 | 1.00 | 12.85 | A |
| ATOM | 1314 | CD2 | LEU | A | 179 | 37.134 | 37.692 | 50.787 | 1.00 | 15.70 | A |
| ATOM | 1315 | C   | LEU | A | 179 | 38.986 | 38.779 | 54.555 | 1.00 | 12.52 | A |
| ATOM | 1316 | O   | LEU | A | 179 | 40.096 | 38.319 | 54.233 | 1.00 | 13.43 | A |
| ATOM | 1317 | N   | SER | A | 180 | 38.788 | 39.426 | 55.702 | 1.00 | 13.88 | A |
| ATOM | 1318 | CA  | SER | A | 180 | 39.910 | 39.635 | 56.612 | 1.00 | 17.84 | A |
| ATOM | 1319 | CB  | SER | A | 180 | 39.438 | 40.187 | 57.954 | 1.00 | 23.37 | A |
| ATOM | 1320 | OG  | SER | A | 180 | 39.006 | 41.521 | 57.770 | 1.00 | 30.75 | A |
| ATOM | 1321 | C   | SER | A | 180 | 40.776 | 38.411 | 56.839 | 1.00 | 18.97 | A |
| ATOM | 1322 | O   | SER | A | 180 | 41.990 | 38.527 | 56.856 | 1.00 | 16.57 | A |
| ATOM | 1323 | N   | PRO | A | 181 | 40.170 | 37.223 | 57.010 | 1.00 | 17.96 | A |
| ATOM | 1324 | CD  | PRO | A | 181 | 38.739 | 36.923 | 57.219 | 1.00 | 18.24 | A |
| ATOM | 1325 | CA  | PRO | A | 181 | 40.989 | 36.023 | 57.228 | 1.00 | 19.35 | A |
| ATOM | 1326 | CB  | PRO | A | 181 | 39.948 | 34.925 | 57.436 | 1.00 | 20.22 | A |
| ATOM | 1327 | CG  | PRO | A | 181 | 38.804 | 35.657 | 58.063 | 1.00 | 20.57 | A |
| ATOM | 1328 | C   | PRO | A | 181 | 41.927 | 35.697 | 56.063 | 1.00 | 24.47 | A |
| ATOM | 1329 | O   | PRO | A | 181 | 42.893 | 34.943 | 56.237 | 1.00 | 26.18 | A |
| ATOM | 1330 | N   | LEU | A | 182 | 41.646 | 36.251 | 54.880 | 1.00 | 17.84 | A |
| ATOM | 1331 | CA  | LEU | A | 182 | 42.470 | 36.002 | 53.688 | 1.00 | 21.43 | A |
| ATOM | 1332 | CB  | LEU | A | 182 | 41.615 | 36.019 | 52.410 | 1.00 | 20.15 | A |
| ATOM | 1333 | CG  | LEU | A | 182 | 40.748 | 34.780 | 52.178 | 1.00 | 20.14 | A |
| ATOM | 1334 | CD1 | LEU | A | 182 | 39.849 | 34.968 | 50.952 | 1.00 | 17.30 | A |
| ATOM | 1335 | CD2 | LEU | A | 182 | 41.679 | 33.580 | 52.004 | 1.00 | 15.09 | A |
| ATOM | 1336 | C   | LEU | A | 182 | 43.614 | 36.985 | 53.490 | 1.00 | 27.88 | A |
| ATOM | 1337 | O   | LEU | A | 182 | 43.499 | 37.909 | 52.682 | 1.00 | 31.51 | A |
| ATOM | 1338 | N   | ALA | A | 183 | 44.726 | 36.761 | 54.185 | 1.00 | 23.49 | A |
| ATOM | 1339 | CA  | ALA | A | 183 | 45.893 | 37.639 | 54.073 | 1.00 | 26.24 | A |
| ATOM | 1340 | CB  | ALA | A | 183 | 47.066 | 37.047 | 54.860 | 1.00 | 22.25 | A |
| ATOM | 1341 | C   | ALA | A | 183 | 46.325 | 37.920 | 52.629 | 1.00 | 20.58 | A |
| ATOM | 1342 | O   | ALA | A | 183 | 46.623 | 37.001 | 51.856 | 1.00 | 17.37 | A |
| ATOM | 1343 | N   | GLY | A | 184 | 46.354 | 39.202 | 52.278 | 1.00 | 17.97 | A |
| ATOM | 1344 | CA  | GLY | A | 184 | 46.762 | 39.603 | 50.949 | 1.00 | 17.46 | A |
| ATOM | 1345 | C   | GLY | A | 184 | 45.908 | 39.186 | 49.755 | 1.00 | 12.78 | A |
| ATOM | 1346 | O   | GLY | A | 184 | 46.413 | 39.159 | 48.636 | 1.00 | 15.39 | A |
| ATOM | 1347 | N   | ALA | A | 185 | 44.634 | 38.878 | 49.956 | 1.00 | 12.15 | A |
| ATOM | 1348 | CA  | ALA | A | 185 | 43.798 | 38.500 | 48.811 | 1.00 | 14.55 | A |
| ATOM | 1349 | CB  | ALA | A | 185 | 42.374 | 38.212 | 49.271 | 1.00 | 14.22 | A |
| ATOM | 1350 | C   | ALA | A | 185 | 43.812 | 39.649 | 47.795 | 1.00 | 16.74 | A |
| ATOM | 1351 | O   | ALA | A | 185 | 43.780 | 40.826 | 48.181 | 1.00 | 15.66 | A |
| ATOM | 1352 | N   | VAL | A | 186 | 43.836 | 39.300 | 46.507 | 1.00 | 9.90  | A |
| ATOM | 1353 | CA  | VAL | A | 186 | 43.880 | 40.276 | 45.419 | 1.00 | 11.92 | A |
| ATOM | 1354 | CB  | VAL | A | 186 | 45.093 | 39.969 | 44.484 | 1.00 | 14.98 | A |
| ATOM | 1355 | CG1 | VAL | A | 186 | 45.026 | 40.816 | 43.229 | 1.00 | 13.29 | A |
| ATOM | 1356 | CG2 | VAL | A | 186 | 46.398 | 40.226 | 45.244 | 1.00 | 19.64 | A |
| ATOM | 1357 | C   | VAL | A | 186 | 42.608 | 40.254 | 44.571 | 1.00 | 11.79 | A |
| ATOM | 1358 | O   | VAL | A | 186 | 42.152 | 39.182 | 44.149 | 1.00 | 11.34 | A |
| ATOM | 1359 | N   | ALA | A | 187 | 42.035 | 41.430 | 44.331 | 1.00 | 11.06 | A |
| ATOM | 1360 | CA  | ALA | A | 187 | 40.829 | 41.543 | 43.508 | 1.00 | 10.57 | A |
| ATOM | 1361 | CB  | ALA | A | 187 | 39.897 | 42.606 | 44.096 | 1.00 | 12.53 | A |
| ATOM | 1362 | C   | ALA | A | 187 | 41.211 | 41.923 | 42.079 | 1.00 | 13.16 | A |
| ATOM | 1363 | O   | ALA | A | 187 | 42.128 | 42.736 | 41.876 | 1.00 | 14.58 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1364 | N   | ALA | A | 188 | 40.543 | 41.328 | 41.085 | 1.00 | 8.38  | A |
| ATOM | 1365 | CA  | ALA | A | 188 | 40.832 | 41.672 | 39.672 | 1.00 | 8.09  | A |
| ATOM | 1366 | CB  | ALA | A | 188 | 41.725 | 40.609 | 39.018 | 1.00 | 10.94 | A |
| ATOM | 1367 | C   | ALA | A | 188 | 39.515 | 41.759 | 38.913 | 1.00 | 9.75  | A |
| ATOM | 1368 | O   | ALA | A | 188 | 38.510 | 41.196 | 39.349 | 1.00 | 10.74 | A |
| ATOM | 1369 | N   | ILE | A | 189 | 39.543 | 42.434 | 37.766 | 1.00 | 10.19 | A |
| ATOM | 1370 | CA  | ILE | A | 189 | 38.355 | 42.646 | 36.936 | 1.00 | 9.71  | A |
| ATOM | 1371 | CB  | ILE | A | 189 | 38.300 | 44.126 | 36.487 | 1.00 | 14.84 | A |
| ATOM | 1372 | CG2 | ILE | A | 189 | 37.056 | 44.394 | 35.606 | 1.00 | 12.56 | A |
| ATOM | 1373 | CG1 | ILE | A | 189 | 38.247 | 45.007 | 37.720 | 1.00 | 13.85 | A |
| ATOM | 1374 | CD1 | ILE | A | 189 | 36.964 | 44.848 | 38.520 | 1.00 | 20.17 | A |
| ATOM | 1375 | C   | ILE | A | 189 | 38.307 | 41.760 | 35.705 | 1.00 | 11.18 | A |
| ATOM | 1376 | O   | ILE | A | 189 | 39.260 | 41.715 | 34.930 | 1.00 | 12.80 | A |
| ATOM | 1377 | N   | GLY | A | 190 | 37.185 | 41.062 | 35.518 | 1.00 | 12.93 | A |
| ATOM | 1378 | CA  | GLY | A | 190 | 37.039 | 40.181 | 34.368 | 1.00 | 9.66  | A |
| ATOM | 1379 | C   | GLY | A | 190 | 37.836 | 38.881 | 34.432 | 1.00 | 11.20 | A |
| ATOM | 1380 | O   | GLY | A | 190 | 38.763 | 38.745 | 35.238 | 1.00 | 12.00 | A |
| ATOM | 1381 | N   | SER | A | 191 | 37.494 | 37.919 | 33.570 | 1.00 | 12.31 | A |
| ATOM | 1382 | CA  | SER | A | 191 | 38.216 | 36.644 | 33.539 | 1.00 | 11.69 | A |
| ATOM | 1383 | CB  | SER | A | 191 | 37.530 | 35.671 | 32.568 | 1.00 | 8.59  | A |
| ATOM | 1384 | OG  | SER | A | 191 | 36.224 | 35.299 | 33.026 | 1.00 | 10.08 | A |
| ATOM | 1385 | C   | SER | A | 191 | 39.678 | 36.896 | 33.104 | 1.00 | 14.30 | A |
| ATOM | 1386 | O   | SER | A | 191 | 40.612 | 36.295 | 33.638 | 1.00 | 11.39 | A |
| ATOM | 1387 | N   | VAL | A | 192 | 39.880 | 37.809 | 32.156 | 1.00 | 11.76 | A |
| ATOM | 1388 | CA  | VAL | A | 192 | 41.235 | 38.101 | 31.704 | 1.00 | 14.84 | A |
| ATOM | 1389 | CB  | VAL | A | 192 | 41.273 | 39.029 | 30.449 | 1.00 | 13.34 | A |
| ATOM | 1390 | CG1 | VAL | A | 192 | 40.838 | 38.252 | 29.213 | 1.00 | 24.13 | A |
| ATOM | 1391 | CG2 | VAL | A | 192 | 40.396 | 40.246 | 30.678 | 1.00 | 29.05 | A |
| ATOM | 1392 | C   | VAL | A | 192 | 42.056 | 38.767 | 32.804 | 1.00 | 11.65 | A |
| ATOM | 1393 | O   | VAL | A | 192 | 43.247 | 38.485 | 32.940 | 1.00 | 14.10 | A |
| ATOM | 1394 | N   | GLY | A | 193 | 41.431 | 39.670 | 33.559 | 1.00 | 12.08 | A |
| ATOM | 1395 | CA  | GLY | A | 193 | 42.149 | 40.344 | 34.626 | 1.00 | 12.16 | A |
| ATOM | 1396 | C   | GLY | A | 193 | 42.575 | 39.354 | 35.700 | 1.00 | 14.30 | A |
| ATOM | 1397 | O   | GLY | A | 193 | 43.652 | 39.486 | 36.291 | 1.00 | 9.20  | A |
| ATOM | 1398 | N   | VAL | A | 194 | 41.725 | 38.369 | 35.976 | 1.00 | 9.32  | A |
| ATOM | 1399 | CA  | VAL | A | 194 | 42.069 | 37.370 | 36.992 | 1.00 | 9.16  | A |
| ATOM | 1400 | CB  | VAL | A | 194 | 40.845 | 36.459 | 37.341 | 1.00 | 7.74  | A |
| ATOM | 1401 | CG1 | VAL | A | 194 | 41.309 | 35.168 | 38.071 | 1.00 | 8.55  | A |
| ATOM | 1402 | CG2 | VAL | A | 194 | 39.873 | 37.247 | 38.259 | 1.00 | 11.33 | A |
| ATOM | 1403 | C   | VAL | A | 194 | 43.256 | 36.524 | 36.530 | 1.00 | 10.65 | A |
| ATOM | 1404 | O   | VAL | A | 194 | 44.158 | 36.255 | 37.318 | 1.00 | 10.00 | A |
| ATOM | 1405 | N   | MET | A | 195 | 43.261 | 36.090 | 35.265 | 1.00 | 9.82  | A |
| ATOM | 1406 | CA  | MET | A | 195 | 44.391 | 35.306 | 34.775 | 1.00 | 11.27 | A |
| ATOM | 1407 | CB  | MET | A | 195 | 44.125 | 34.727 | 33.381 | 1.00 | 13.33 | A |
| ATOM | 1408 | CG  | MET | A | 195 | 43.342 | 33.449 | 33.381 | 1.00 | 16.98 | A |
| ATOM | 1409 | SD  | MET | A | 195 | 43.794 | 32.237 | 34.698 | 1.00 | 19.79 | A |
| ATOM | 1410 | CE  | MET | A | 195 | 45.205 | 31.419 | 34.043 | 1.00 | 16.46 | A |
| ATOM | 1411 | C   | MET | A | 195 | 45.672 | 36.118 | 34.719 | 1.00 | 12.67 | A |
| ATOM | 1412 | O   | MET | A | 195 | 46.757 | 35.579 | 34.948 | 1.00 | 15.56 | A |
| ATOM | 1413 | N   | ALA | A | 196 | 45.566 | 37.401 | 34.385 | 1.00 | 11.82 | A |
| ATOM | 1414 | CA  | ALA | A | 196 | 46.750 | 38.239 | 34.346 | 1.00 | 15.74 | A |
| ATOM | 1415 | CB  | ALA | A | 196 | 46.404 | 39.633 | 33.833 | 1.00 | 14.20 | A |
| ATOM | 1416 | C   | ALA | A | 196 | 47.331 | 38.323 | 35.768 | 1.00 | 16.81 | A |
| ATOM | 1417 | O   | ALA | A | 196 | 48.544 | 38.245 | 35.945 | 1.00 | 15.03 | A |
| ATOM | 1418 | N   | ALA | A | 197 | 46.464 | 38.468 | 36.778 | 1.00 | 13.86 | A |
| ATOM | 1419 | CA  | ALA | A | 197 | 46.939 | 38.538 | 38.151 | 1.00 | 13.25 | A |
| ATOM | 1420 | CB  | ALA | A | 197 | 45.790 | 38.865 | 39.108 | 1.00 | 13.70 | A |
| ATOM | 1421 | C   | ALA | A | 197 | 47.547 | 37.203 | 38.542 | 1.00 | 13.49 | A |
| ATOM | 1422 | O   | ALA | A | 197 | 48.618 | 37.159 | 39.147 | 1.00 | 13.32 | A |
| ATOM | 1423 | N   | ASP | A | 198 | 46.853 | 36.119 | 38.202 | 1.00 | 12.41 | A |
| ATOM | 1424 | CA  | ASP | A | 198 | 47.326 | 34.777 | 38.547 | 1.00 | 16.61 | A |
| ATOM | 1425 | CB  | ASP | A | 198 | 46.311 | 33.719 | 38.074 | 1.00 | 18.96 | A |
| ATOM | 1426 | CG  | ASP | A | 198 | 46.605 | 32.327 | 38.629 | 1.00 | 29.19 | A |
| ATOM | 1427 | OD1 | ASP | A | 198 | 46.440 | 32.107 | 39.857 | 1.00 | 32.24 | A |
| ATOM | 1428 | OD2 | ASP | A | 198 | 47.004 | 31.449 | 37.834 | 1.00 | 34.04 | A |
| ATOM | 1429 | C   | ASP | A | 198 | 48.699 | 34.509 | 37.928 | 1.00 | 17.95 | A |
| ATOM | 1430 | O   | ASP | A | 198 | 49.570 | 33.942 | 38.585 | 1.00 | 18.27 | A |
| ATOM | 1431 | N   | ASN | A | 199 | 48.900 | 34.941 | 36.684 | 1.00 | 16.24 | A |
| ATOM | 1432 | CA  | ASN | A | 199 | 50.173 | 34.733 | 35.980 | 1.00 | 17.75 | A |
| ATOM | 1433 | CB  | ASN | A | 199 | 49.941 | 34.565 | 34.478 | 1.00 | 19.50 | A |
| ATOM | 1434 | CG  | ASN | A | 199 | 49.270 | 33.263 | 34.122 | 1.00 | 21.16 | A |
| ATOM | 1435 | OD1 | ASN | A | 199 | 49.454 | 32.254 | 34.786 | 1.00 | 29.31 | A |
| ATOM | 1436 | ND2 | ASN | A | 199 | 48.504 | 33.275 | 33.041 | 1.00 | 24.39 | A |
| ATOM | 1437 | C   | ASN | A | 199 | 51.227 | 35.832 | 36.144 | 1.00 | 20.64 | A |
| ATOM | 1438 | O   | ASN | A | 199 | 52.272 | 35.762 | 35.507 | 1.00 | 27.47 | A |
| ATOM | 1439 | N   | ASP | A | 200 | 50.973 | 36.838 | 36.970 | 1.00 | 19.22 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1440 | CA  | ASP | A | 200 | 51.925 | 37.937 | 37.148 | 1.00 | 20.54 | A |
| ATOM | 1441 | CB  | ASP | A | 200 | 51.350 | 38.985 | 38.092 | 1.00 | 22.32 | A |
| ATOM | 1442 | CG  | ASP | A | 200 | 52.166 | 40.271 | 38.105 | 1.00 | 23.11 | A |
| ATOM | 1443 | OD1 | ASP | A | 200 | 53.356 | 40.256 | 37.713 | 1.00 | 21.11 | A |
| ATOM | 1444 | OD2 | ASP | A | 200 | 51.612 | 41.296 | 38.526 | 1.00 | 26.57 | A |
| ATOM | 1445 | C   | ASP | A | 200 | 53.252 | 37.431 | 37.716 | 1.00 | 21.98 | A |
| ATOM | 1446 | O   | ASP | A | 200 | 53.315 | 36.967 | 38.855 | 1.00 | 19.25 | A |
| ATOM | 1447 | N   | VAL | A | 201 | 54.315 | 37.511 | 36.922 | 1.00 | 21.71 | A |
| ATOM | 1448 | CA  | VAL | A | 201 | 55.611 | 37.033 | 37.390 | 1.00 | 24.01 | A |
| ATOM | 1449 | CB  | VAL | A | 201 | 56.519 | 36.597 | 36.216 | 1.00 | 23.59 | A |
| ATOM | 1450 | CG1 | VAL | A | 201 | 55.910 | 35.377 | 35.519 | 1.00 | 25.93 | A |
| ATOM | 1451 | CG2 | VAL | A | 201 | 56.710 | 37.754 | 35.246 | 1.00 | 26.53 | A |
| ATOM | 1452 | C   | VAL | A | 201 | 56.370 | 38.046 | 38.222 | 1.00 | 24.27 | A |
| ATOM | 1453 | O   | VAL | A | 201 | 57.451 | 37.744 | 38.715 | 1.00 | 30.90 | A |
| ATOM | 1454 | N   | THR | A | 202 | 55.817 | 39.241 | 38.402 | 1.00 | 23.14 | A |
| ATOM | 1455 | CA  | THR | A | 202 | 56.511 | 40.251 | 39.190 | 1.00 | 23.53 | A |
| ATOM | 1456 | CB  | THR | A | 202 | 56.216 | 41.664 | 38.696 | 1.00 | 22.33 | A |
| ATOM | 1457 | OG1 | THR | A | 202 | 54.846 | 41.999 | 38.979 | 1.00 | 24.30 | A |
| ATOM | 1458 | CG2 | THR | A | 202 | 56.489 | 41.759 | 37.210 | 1.00 | 25.94 | A |
| ATOM | 1459 | C   | THR | A | 202 | 56.171 | 40.184 | 40.677 | 1.00 | 24.49 | A |
| ATOM | 1460 | O   | THR | A | 202 | 56.543 | 41.073 | 41.444 | 1.00 | 25.68 | A |
| ATOM | 1461 | N   | THR | A | 203 | 55.440 | 39.147 | 41.076 | 1.00 | 19.97 | A |
| ATOM | 1462 | CA  | THR | A | 203 | 55.116 | 38.957 | 42.484 | 1.00 | 20.69 | A |
| ATOM | 1463 | CB  | THR | A | 203 | 53.608 | 39.167 | 42.768 | 1.00 | 26.13 | A |
| ATOM | 1464 | OG1 | THR | A | 203 | 52.825 | 38.196 | 42.047 | 1.00 | 25.13 | A |
| ATOM | 1465 | CG2 | THR | A | 203 | 53.202 | 40.581 | 42.363 | 1.00 | 26.59 | A |
| ATOM | 1466 | C   | THR | A | 203 | 55.523 | 37.521 | 42.834 | 1.00 | 17.47 | A |
| ATOM | 1467 | O   | THR | A | 203 | 56.771 | 36.703 | 41.947 | 1.00 | 18.21 | A |
| ATOM | 1468 | N   | ALA | A | 204 | 55.624 | 37.217 | 44.116 | 1.00 | 16.96 | A |
| ATOM | 1469 | CA  | ALA | A | 204 | 56.011 | 35.867 | 44.528 | 1.00 | 16.26 | A |
| ATOM | 1470 | CB  | ALA | A | 204 | 56.175 | 35.825 | 46.065 | 1.00 | 18.50 | A |
| ATOM | 1471 | C   | ALA | A | 204 | 54.978 | 34.832 | 44.092 | 1.00 | 14.92 | A |
| ATOM | 1472 | O   | ALA | A | 204 | 53.806 | 35.157 | 43.906 | 1.00 | 16.09 | A |
| ATOM | 1473 | N   | GLN | A | 205 | 55.409 | 33.582 | 43.921 | 1.00 | 16.21 | A |
| ATOM | 1474 | CA  | GLN | A | 205 | 54.483 | 32.501 | 43.560 | 1.00 | 16.27 | A |
| ATOM | 1475 | CB  | GLN | A | 205 | 55.232 | 31.191 | 43.316 | 1.00 | 15.65 | A |
| ATOM | 1476 | CG  | GLN | A | 205 | 56.103 | 31.148 | 42.097 | 1.00 | 22.41 | A |
| ATOM | 1477 | CD  | GLN | A | 205 | 56.469 | 29.716 | 41.717 | 1.00 | 29.28 | A |
| ATOM | 1478 | OE1 | GLN | A | 205 | 56.446 | 28.801 | 42.565 | 1.00 | 20.67 | A |
| ATOM | 1479 | NE2 | GLN | A | 205 | 56.813 | 29.510 | 40.442 | 1.00 | 25.77 | A |
| ATOM | 1480 | C   | GLN | A | 205 | 53.529 | 32.262 | 44.728 | 1.00 | 14.53 | A |
| ATOM | 1481 | O   | GLN | A | 205 | 53.783 | 32.717 | 45.846 | 1.00 | 14.81 | A |
| ATOM | 1482 | N   | GLY | A | 206 | 52.438 | 31.540 | 44.478 | 1.00 | 11.64 | A |
| ATOM | 1483 | CA  | GLY | A | 206 | 51.509 | 31.236 | 45.554 | 1.00 | 11.46 | A |
| ATOM | 1484 | C   | GLY | A | 206 | 50.042 | 31.518 | 45.284 | 1.00 | 11.44 | A |
| ATOM | 1485 | O   | GLY | A | 206 | 49.162 | 31.067 | 46.046 | 1.00 | 9.87  | A |
| ATOM | 1486 | N   | ARG | A | 207 | 49.764 | 32.236 | 44.199 | 1.00 | 7.71  | A |
| ATOM | 1487 | CA  | ARG | A | 207 | 48.383 | 32.606 | 43.878 | 1.00 | 7.50  | A |
| ATOM | 1488 | CB  | ARG | A | 207 | 48.364 | 33.763 | 42.863 | 1.00 | 9.66  | A |
| ATOM | 1489 | CG  | ARG | A | 207 | 48.719 | 35.114 | 43.493 | 1.00 | 7.35  | A |
| ATOM | 1490 | CD  | ARG | A | 207 | 48.774 | 36.286 | 42.497 | 1.00 | 6.76  | A |
| ATOM | 1491 | NE  | ARG | A | 207 | 49.079 | 37.532 | 43.221 | 1.00 | 10.86 | A |
| ATOM | 1492 | CZ  | ARG | A | 207 | 49.156 | 38.738 | 42.654 | 1.00 | 13.78 | A |
| ATOM | 1493 | NH1 | ARG | A | 207 | 48.957 | 38.881 | 41.350 | 1.00 | 9.77  | A |
| ATOM | 1494 | NH2 | ARG | A | 207 | 49.415 | 39.811 | 43.398 | 1.00 | 15.04 | A |
| ATOM | 1495 | C   | ARG | A | 207 | 47.500 | 31.475 | 43.389 | 1.00 | 11.20 | A |
| ATOM | 1496 | O   | ARG | A | 207 | 47.959 | 30.549 | 42.713 | 1.00 | 12.10 | A |
| ATOM | 1497 | N   | ILE | A | 208 | 46.214 | 31.572 | 43.721 | 1.00 | 8.65  | A |
| ATOM | 1498 | CA  | ILE | A | 208 | 45.245 | 30.557 | 43.331 | 1.00 | 8.62  | A |
| ATOM | 1499 | CB  | ILE | A | 208 | 45.073 | 29.491 | 44.476 | 1.00 | 11.42 | A |
| ATOM | 1500 | CG2 | ILE | A | 208 | 44.533 | 30.157 | 45.766 | 1.00 | 8.84  | A |
| ATOM | 1501 | CG1 | ILE | A | 208 | 44.158 | 28.359 | 43.984 | 1.00 | 12.09 | A |
| ATOM | 1502 | CD1 | ILE | A | 208 | 44.207 | 27.094 | 44.823 | 1.00 | 11.77 | A |
| ATOM | 1503 | C   | ILE | A | 208 | 43.924 | 31.286 | 43.056 | 1.00 | 10.31 | A |
| ATOM | 1504 | O   | ILE | A | 208 | 43.664 | 32.335 | 43.649 | 1.00 | 12.81 | A |
| ATOM | 1505 | N   | THR | A | 209 | 43.098 | 30.776 | 42.145 | 1.00 | 7.78  | A |
| ATOM | 1506 | CA  | THR | A | 209 | 41.825 | 31.470 | 41.864 | 1.00 | 9.01  | A |
| ATOM | 1507 | CB  | THR | A | 209 | 42.055 | 32.610 | 40.849 | 1.00 | 11.48 | A |
| ATOM | 1508 | OG1 | THR | A | 209 | 40.906 | 33.455 | 40.789 | 1.00 | 11.18 | A |
| ATOM | 1509 | CG2 | THR | A | 209 | 42.310 | 32.030 | 39.460 | 1.00 | 12.27 | A |
| ATOM | 1510 | C   | THR | A | 209 | 40.751 | 30.534 | 41.319 | 1.00 | 10.48 | A |
| ATOM | 1511 | O   | THR | A | 209 | 40.978 | 29.326 | 41.215 | 1.00 | 10.85 | A |
| ATOM | 1512 | N   | TYR | A | 210 | 39.577 | 31.087 | 40.997 | 1.00 | 8.58  | A |
| ATOM | 1513 | CA  | TYR | A | 210 | 38.476 | 30.303 | 40.422 | 1.00 | 8.34  | A |
| ATOM | 1514 | CB  | TYR | A | 210 | 37.244 | 30.304 | 41.350 | 1.00 | 4.35  | A |
| ATOM | 1515 | CG  | TYR | A | 210 | 36.685 | 31.664 | 41.695 | 1.00 | 7.98  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1516 | CD1 | TYR | A | 210 | 35.656 | 32.240 | 40.927 | 1.00 | 6.11  | A |
| ATOM | 1517 | CE1 | TYR | A | 210 | 35.153 | 33.509 | 41.235 | 1.00 | 7.73  | A |
| ATOM | 1518 | CD2 | TYR | A | 210 | 37.188 | 32.386 | 42.778 | 1.00 | 6.57  | A |
| ATOM | 1519 | CE2 | TYR | A | 210 | 36.699 | 33.643 | 43.086 | 1.00 | 5.93  | A |
| ATOM | 1520 | CZ  | TYR | A | 210 | 35.687 | 34.203 | 42.313 | 1.00 | 8.47  | A |
| ATOM | 1521 | OH  | TYR | A | 210 | 35.242 | 35.475 | 42.598 | 1.00 | 8.24  | A |
| ATOM | 1522 | C   | TYR | A | 210 | 38.169 | 30.983 | 39.087 | 1.00 | 5.52  | A |
| ATOM | 1523 | O   | TYR | A | 210 | 38.184 | 32.222 | 39.010 | 1.00 | 9.37  | A |
| ATOM | 1524 | N   | ILE | A | 211 | 37.934 | 30.201 | 38.032 | 1.00 | 6.28  | A |
| ATOM | 1525 | CA  | ILE | A | 211 | 37.720 | 30.832 | 36.735 | 1.00 | 7.52  | A |
| ATOM | 1526 | CB  | ILE | A | 211 | 39.085 | 31.384 | 36.235 | 1.00 | 11.97 | A |
| ATOM | 1527 | CG2 | ILE | A | 211 | 39.990 | 30.231 | 35.830 | 1.00 | 10.21 | A |
| ATOM | 1528 | CG1 | ILE | A | 211 | 38.902 | 32.361 | 35.075 | 1.00 | 14.62 | A |
| ATOM | 1529 | CD1 | ILE | A | 211 | 40.159 | 33.203 | 34.806 | 1.00 | 15.71 | A |
| ATOM | 1530 | C   | ILE | A | 211 | 37.132 | 29.936 | 35.648 | 1.00 | 8.22  | A |
| ATOM | 1531 | O   | ILE | A | 211 | 37.080 | 28.703 | 35.778 | 1.00 | 8.13  | A |
| ATOM | 1532 | N   | SER | A | 212 | 36.634 | 30.590 | 34.602 | 1.00 | 9.06  | A |
| ATOM | 1533 | CA  | SER | A | 212 | 36.140 | 29.913 | 33.394 | 1.00 | 9.98  | A |
| ATOM | 1534 | CB  | SER | A | 212 | 35.984 | 30.934 | 32.256 | 1.00 | 8.45  | A |
| ATOM | 1535 | OG  | SER | A | 212 | 35.637 | 30.283 | 31.037 | 1.00 | 9.53  | A |
| ATOM | 1536 | C   | SER | A | 212 | 37.181 | 28.904 | 32.914 | 1.00 | 10.00 | A |
| ATOM | 1537 | O   | SER | A | 212 | 38.361 | 29.234 | 32.812 | 1.00 | 7.50  | A |
| ATOM | 1538 | N   | PRO | A | 213 | 36.761 | 27.668 | 32.585 | 1.00 | 8.50  | A |
| ATOM | 1539 | CD  | PRO | A | 213 | 35.436 | 27.030 | 32.686 | 1.00 | 4.78  | A |
| ATOM | 1540 | CA  | PRO | A | 213 | 37.781 | 26.728 | 32.117 | 1.00 | 8.39  | A |
| ATOM | 1541 | CB  | PRO | A | 213 | 37.035 | 25.392 | 32.059 | 1.00 | 10.29 | A |
| ATOM | 1542 | CG  | PRO | A | 213 | 35.578 | 25.849 | 31.743 | 1.00 | 9.33  | A |
| ATOM | 1543 | C   | PRO | A | 213 | 38.360 | 27.149 | 30.777 | 1.00 | 10.79 | A |
| ATOM | 1544 | O   | PRO | A | 213 | 39.433 | 26.698 | 30.390 | 1.00 | 10.83 | A |
| ATOM | 1545 | N   | ASP | A | 214 | 37.668 | 28.038 | 30.074 | 1.00 | 5.80  | A |
| ATOM | 1546 | CA  | ASP | A | 214 | 38.164 | 28.514 | 28.775 | 1.00 | 8.50  | A |
| ATOM | 1547 | CB  | ASP | A | 214 | 37.033 | 29.175 | 27.997 | 1.00 | 7.35  | A |
| ATOM | 1548 | CG  | ASP | A | 214 | 37.248 | 29.146 | 26.497 | 1.00 | 11.12 | A |
| ATOM | 1549 | OD1 | ASP | A | 214 | 36.479 | 29.849 | 25.801 | 1.00 | 11.42 | A |
| ATOM | 1550 | OD2 | ASP | A | 214 | 38.159 | 28.428 | 26.007 | 1.00 | 10.72 | A |
| ATOM | 1551 | C   | ASP | A | 214 | 39.314 | 29.526 | 28.935 | 1.00 | 12.08 | A |
| ATOM | 1552 | O   | ASP | A | 214 | 39.933 | 29.931 | 27.943 | 1.00 | 13.08 | A |
| ATOM | 1553 | N   | PHE | A | 215 | 39.572 | 29.958 | 30.170 | 1.00 | 9.47  | A |
| ATOM | 1554 | CA  | PHE | A | 215 | 40.662 | 30.901 | 30.459 | 1.00 | 9.63  | A |
| ATOM | 1555 | CB  | PHE | A | 215 | 40.121 | 32.106 | 31.233 | 1.00 | 12.63 | A |
| ATOM | 1556 | CG  | PHE | A | 215 | 39.375 | 33.081 | 30.402 | 1.00 | 9.86  | A |
| ATOM | 1557 | CD1 | PHE | A | 215 | 39.957 | 34.301 | 30.067 | 1.00 | 11.72 | A |
| ATOM | 1558 | CD2 | PHE | A | 215 | 38.074 | 32.812 | 29.985 | 1.00 | 11.34 | A |
| ATOM | 1559 | CE1 | PHE | A | 215 | 39.250 | 35.250 | 29.332 | 1.00 | 11.89 | A |
| ATOM | 1560 | CE2 | PHE | A | 215 | 37.357 | 33.759 | 29.245 | 1.00 | 6.37  | A |
| ATOM | 1561 | CZ  | PHE | A | 215 | 37.949 | 34.976 | 28.921 | 1.00 | 13.90 | A |
| ATOM | 1562 | C   | PHE | A | 215 | 41.748 | 30.286 | 31.356 | 1.00 | 13.88 | A |
| ATOM | 1563 | O   | PHE | A | 215 | 42.837 | 30.865 | 31.480 | 1.00 | 12.28 | A |
| ATOM | 1564 | N   | ALA | A | 216 | 41.463 | 29.131 | 31.976 | 1.00 | 9.02  | A |
| ATOM | 1565 | CA  | ALA | A | 216 | 42.404 | 28.535 | 32.936 | 1.00 | 9.41  | A |
| ATOM | 1566 | CB  | ALA | A | 216 | 41.705 | 27.432 | 33.753 | 1.00 | 9.18  | A |
| ATOM | 1567 | C   | ALA | A | 216 | 43.727 | 28.007 | 32.406 | 1.00 | 13.18 | A |
| ATOM | 1568 | O   | ALA | A | 216 | 44.679 | 27.844 | 33.178 | 1.00 | 16.82 | A |
| ATOM | 1569 | N   | ALA | A | 217 | 43.790 | 27.719 | 31.106 | 1.00 | 12.39 | A |
| ATOM | 1570 | CA  | ALA | A | 217 | 45.031 | 27.224 | 30.522 | 1.00 | 14.59 | A |
| ATOM | 1571 | CB  | ALA | A | 217 | 45.094 | 25.693 | 30.625 | 1.00 | 15.34 | A |
| ATOM | 1572 | C   | ALA | A | 217 | 45.136 | 27.660 | 29.063 | 1.00 | 16.52 | A |
| ATOM | 1573 | O   | ALA | A | 217 | 44.128 | 27.958 | 28.418 | 1.00 | 14.71 | A |
| ATOM | 1574 | N   | PRO | A | 218 | 46.358 | 27.690 | 28.517 | 1.00 | 18.85 | A |
| ATOM | 1575 | CD  | PRO | A | 218 | 47.657 | 27.532 | 29.194 | 1.00 | 19.53 | A |
| ATOM | 1576 | CA  | PRO | A | 218 | 46.533 | 28.101 | 27.111 | 1.00 | 17.17 | A |
| ATOM | 1577 | CB  | PRO | A | 218 | 48.053 | 28.171 | 26.952 | 1.00 | 22.03 | A |
| ATOM | 1578 | CG  | PRO | A | 218 | 48.553 | 28.433 | 28.357 | 1.00 | 24.10 | A |
| ATOM | 1579 | C   | PRO | A | 218 | 45.889 | 27.162 | 26.076 | 1.00 | 17.95 | A |
| ATOM | 1580 | O   | PRO | A | 218 | 45.490 | 27.606 | 24.986 | 1.00 | 20.60 | A |
| ATOM | 1581 | N   | SER | A | 219 | 45.804 | 25.872 | 26.395 | 1.00 | 12.39 | A |
| ATOM | 1582 | CA  | SER | A | 219 | 45.212 | 24.883 | 25.490 | 1.00 | 11.61 | A |
| ATOM | 1583 | CB  | SER | A | 219 | 46.308 | 24.053 | 24.816 | 1.00 | 17.69 | A |
| ATOM | 1584 | OG  | SER | A | 219 | 46.870 | 23.140 | 25.749 | 1.00 | 17.25 | A |
| ATOM | 1585 | C   | SER | A | 219 | 44.341 | 23.942 | 26.324 | 1.00 | 14.52 | A |
| ATOM | 1586 | O   | SER | A | 219 | 44.454 | 23.896 | 27.559 | 1.00 | 15.86 | A |
| ATOM | 1587 | N   | LEU | A | 220 | 43.479 | 23.180 | 25.664 | 1.00 | 13.85 | A |
| ATOM | 1588 | CA  | LEU | A | 220 | 42.614 | 22.250 | 26.389 | 1.00 | 13.63 | A |
| ATOM | 1589 | CB  | LEU | A | 220 | 41.705 | 21.491 | 25.401 | 1.00 | 15.59 | A |
| ATOM | 1590 | CG  | LEU | A | 220 | 40.632 | 22.337 | 24.707 | 1.00 | 16.07 | A |
| ATOM | 1591 | CD1 | LEU | A | 220 | 39.908 | 21.517 | 23.646 | 1.00 | 15.58 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1592 | CD2 | LEU | A | 220 | 39.635 | 22.855 | 25.752 | 1.00 | 16.33 | A |
| ATOM | 1593 | C   | LEU | A | 220 | 43.401 | 21.251 | 27.245 | 1.00 | 15.71 | A |
| ATOM | 1594 | O   | LEU | A | 220 | 43.034 | 20.986 | 28.395 | 1.00 | 15.65 | A |
| ATOM | 1595 | N   | ALA | A | 221 | 44.481 | 20.693 | 26.698 | 1.00 | 15.60 | A |
| ATOM | 1596 | CA  | ALA | A | 221 | 45.283 | 19.714 | 27.452 | 1.00 | 18.03 | A |
| ATOM | 1597 | CB  | ALA | A | 221 | 46.452 | 19.175 | 26.604 | 1.00 | 17.58 | A |
| ATOM | 1598 | C   | ALA | A | 221 | 45.834 | 20.298 | 28.738 | 1.00 | 11.01 | A |
| ATOM | 1599 | O   | ALA | A | 221 | 46.085 | 19.573 | 29.687 | 1.00 | 15.45 | A |
| ATOM | 1600 | N   | GLY | A | 222 | 46.038 | 21.612 | 28.754 | 1.00 | 15.25 | A |
| ATOM | 1601 | CA  | GLY | A | 222 | 46.561 | 22.267 | 29.947 | 1.00 | 11.71 | A |
| ATOM | 1602 | C   | GLY | A | 222 | 45.641 | 22.101 | 31.144 | 1.00 | 10.72 | A |
| ATOM | 1603 | O   | GLY | A | 222 | 46.105 | 22.139 | 32.280 | 1.00 | 14.13 | A |
| ATOM | 1604 | N   | LEU | A | 223 | 44.340 | 21.938 | 30.914 | 1.00 | 11.19 | A |
| ATOM | 1605 | CA  | LEU | A | 223 | 43.406 | 21.751 | 32.033 | 1.00 | 8.14  | A |
| ATOM | 1606 | CB  | LEU | A | 223 | 41.946 | 21.728 | 31.525 | 1.00 | 9.90  | A |
| ATOM | 1607 | CG  | LEU | A | 223 | 41.481 | 23.046 | 30.874 | 1.00 | 9.91  | A |
| ATOM | 1608 | CD1 | LEU | A | 223 | 40.035 | 22.918 | 30.331 | 1.00 | 9.85  | A |
| ATOM | 1609 | CD2 | LEU | A | 223 | 41.570 | 24.153 | 31.926 | 1.00 | 9.05  | A |
| ATOM | 1610 | C   | LEU | A | 223 | 43.720 | 20.444 | 32.773 | 1.00 | 11.22 | A |
| ATOM | 1611 | O   | LEU | A | 223 | 43.369 | 20.297 | 33.939 | 1.00 | 7.21  | A |
| ATOM | 1612 | N   | ASN | A | 224 | 44.389 | 19.505 | 32.100 | 1.00 | 9.60  | A |
| ATOM | 1613 | CA  | ASN | A | 224 | 44.742 | 18.231 | 32.727 | 1.00 | 10.35 | A |
| ATOM | 1614 | CB  | ASN | A | 224 | 44.651 | 17.078 | 31.706 | 1.00 | 13.70 | A |
| ATOM | 1615 | CG  | ASN | A | 224 | 43.214 | 16.768 | 31.301 | 1.00 | 15.75 | A |
| ATOM | 1616 | OD1 | ASN | A | 224 | 42.347 | 16.610 | 32.146 | 1.00 | 21.72 | A |
| ATOM | 1617 | ND2 | ASN | A | 224 | 42.968 | 16.666 | 30.012 | 1.00 | 14.86 | A |
| ATOM | 1618 | C   | ASN | A | 224 | 46.138 | 18.239 | 33.359 | 1.00 | 12.93 | A |
| ATOM | 1619 | O   | ASN | A | 224 | 46.580 | 17.226 | 33.898 | 1.00 | 14.86 | A |
| ATOM | 1620 | N   | ASP | A | 225 | 46.833 | 19.370 | 33.308 | 1.00 | 8.74  | A |
| ATOM | 1621 | CA  | ASP | A | 225 | 48.163 | 19.437 | 33.932 | 1.00 | 12.69 | A |
| ATOM | 1622 | CB  | ASP | A | 225 | 49.031 | 20.467 | 33.199 | 1.00 | 11.40 | A |
| ATOM | 1623 | CG  | ASP | A | 225 | 50.402 | 20.654 | 33.843 | 1.00 | 15.89 | A |
| ATOM | 1624 | OD1 | ASP | A | 225 | 50.673 | 20.076 | 34.922 | 1.00 | 14.10 | A |
| ATOM | 1625 | OD2 | ASP | A | 225 | 51.211 | 21.401 | 33.261 | 1.00 | 16.19 | A |
| ATOM | 1626 | C   | ASP | A | 225 | 47.960 | 19.844 | 35.398 | 1.00 | 13.53 | A |
| ATOM | 1627 | O   | ASP | A | 225 | 47.776 | 21.016 | 35.691 | 1.00 | 10.79 | A |
| ATOM | 1628 | N   | ALA | A | 226 | 48.035 | 18.882 | 36.317 | 1.00 | 10.49 | A |
| ATOM | 1629 | CA  | ALA | A | 226 | 47.792 | 19.178 | 37.720 | 1.00 | 9.18  | A |
| ATOM | 1630 | CB  | ALA | A | 226 | 47.424 | 17.889 | 38.478 | 1.00 | 13.20 | A |
| ATOM | 1631 | C   | ALA | A | 226 | 48.881 | 19.939 | 38.461 | 1.00 | 12.23 | A |
| ATOM | 1632 | O   | ALA | A | 226 | 48.773 | 20.144 | 39.678 | 1.00 | 13.15 | A |
| ATOM | 1633 | N   | THR | A | 227 | 49.935 | 20.347 | 37.762 | 1.00 | 10.64 | A |
| ATOM | 1634 | CA  | THR | A | 227 | 50.955 | 21.148 | 38.426 | 1.00 | 10.50 | A |
| ATOM | 1635 | CB  | THR | A | 227 | 52.405 | 20.854 | 37.917 | 1.00 | 15.63 | A |
| ATOM | 1636 | OG1 | THR | A | 227 | 52.541 | 21.287 | 36.561 | 1.00 | 13.88 | A |
| ATOM | 1637 | CG2 | THR | A | 227 | 52.718 | 19.374 | 38.009 | 1.00 | 16.59 | A |
| ATOM | 1638 | C   | THR | A | 227 | 50.620 | 22.628 | 38.154 | 1.00 | 9.17  | A |
| ATOM | 1639 | O   | THR | A | 227 | 51.320 | 23.509 | 38.626 | 1.00 | 10.52 | A |
| ATOM | 1640 | N   | LYS | A | 228 | 49.530 | 22.876 | 37.414 | 1.00 | 9.27  | A |
| ATOM | 1641 | CA  | LYS | A | 228 | 49.079 | 24.226 | 37.069 | 1.00 | 12.05 | A |
| ATOM | 1642 | CB  | LYS | A | 228 | 49.378 | 24.511 | 35.594 | 1.00 | 15.38 | A |
| ATOM | 1643 | CG  | LYS | A | 228 | 50.877 | 24.607 | 35.272 | 1.00 | 22.71 | A |
| ATOM | 1644 | CD  | LYS | A | 228 | 51.125 | 24.652 | 33.758 | 1.00 | 20.66 | A |
| ATOM | 1645 | CE  | LYS | A | 228 | 52.613 | 24.720 | 33.447 | 1.00 | 26.84 | A |
| ATOM | 1646 | NZ  | LYS | A | 228 | 53.205 | 25.974 | 33.986 | 1.00 | 37.16 | A |
| ATOM | 1647 | C   | LYS | A | 228 | 47.576 | 24.453 | 37.313 | 1.00 | 8.78  | A |
| ATOM | 1648 | O   | LYS | A | 228 | 47.153 | 25.574 | 37.634 | 1.00 | 9.99  | A |
| ATOM | 1649 | N   | VAL | A | 229 | 46.777 | 23.407 | 37.100 | 1.00 | 9.98  | A |
| ATOM | 1650 | CA  | VAL | A | 229 | 45.327 | 23.465 | 37.282 | 1.00 | 6.71  | A |
| ATOM | 1651 | CB  | VAL | A | 229 | 44.611 | 23.300 | 35.939 | 1.00 | 8.87  | A |
| ATOM | 1652 | CG1 | VAL | A | 229 | 43.082 | 23.303 | 36.150 | 1.00 | 10.77 | A |
| ATOM | 1653 | CG2 | VAL | A | 229 | 45.019 | 24.468 | 34.988 | 1.00 | 10.90 | A |
| ATOM | 1654 | C   | VAL | A | 229 | 44.913 | 22.339 | 38.245 | 1.00 | 10.51 | A |
| ATOM | 1655 | O   | VAL | A | 229 | 45.107 | 21.154 | 37.967 | 1.00 | 8.04  | A |
| ATOM | 1656 | N   | ALA | A | 230 | 44.343 | 22.706 | 39.383 | 1.00 | 10.29 | A |
| ATOM | 1657 | CA  | ALA | A | 230 | 43.985 | 21.696 | 40.387 | 1.00 | 8.30  | A |
| ATOM | 1658 | CB  | ALA | A | 230 | 43.612 | 22.380 | 41.677 | 1.00 | 10.71 | A |
| ATOM | 1659 | C   | ALA | A | 230 | 42.900 | 20.691 | 40.064 | 1.00 | 12.18 | A |
| ATOM | 1660 | O   | ALA | A | 230 | 41.884 | 21.020 | 39.435 | 1.00 | 12.58 | A |
| ATOM | 1661 | N   | ARG | A | 231 | 43.120 | 19.452 | 40.501 | 1.00 | 8.23  | A |
| ATOM | 1662 | CA  | ARG | A | 231 | 42.080 | 18.436 | 40.382 | 1.00 | 8.98  | A |
| ATOM | 1663 | CB  | ARG | A | 231 | 42.656 | 17.021 | 40.495 | 1.00 | 11.67 | A |
| ATOM | 1664 | CG  | ARG | A | 231 | 43.433 | 16.581 | 39.265 | 1.00 | 14.58 | A |
| ATOM | 1665 | CD  | ARG | A | 231 | 44.130 | 15.244 | 39.487 | 1.00 | 18.76 | A |
| ATOM | 1666 | NE  | ARG | A | 231 | 44.972 | 14.941 | 38.336 | 1.00 | 19.63 | A |
| ATOM | 1667 | CZ  | ARG | A | 231 | 45.931 | 14.029 | 38.331 | 1.00 | 26.24 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1668 | NH1 | ARG | A | 231 | 46.184 | 13.312 | 39.426 | 1.00 | 22.17 | A |
| ATOM | 1669 | NH2 | ARG | A | 231 | 46.649 | 13.848 | 37.228 | 1.00 | 31.31 | A |
| ATOM | 1670 | C   | ARG | A | 231 | 41.271 | 18.738 | 41.632 | 1.00 | 8.66  | A |
| ATOM | 1671 | O   | ARG | A | 231 | 41.801 | 19.332 | 42.582 | 1.00 | 13.24 | A |
| ATOM | 1672 | N   | THR | A | 232 | 39.997 | 18.371 | 41.640 | 1.00 | 9.11  | A |
| ATOM | 1673 | CA  | THR | A | 232 | 39.180 | 18.607 | 42.822 | 1.00 | 11.84 | A |
| ATOM | 1674 | CB  | THR | A | 232 | 38.236 | 19.820 | 42.623 | 1.00 | 13.64 | A |
| ATOM | 1675 | OG1 | THR | A | 232 | 39.017 | 21.004 | 42.384 | 1.00 | 17.60 | A |
| ATOM | 1676 | CG2 | THR | A | 232 | 37.382 | 20.025 | 43.883 | 1.00 | 14.43 | A |
| ATOM | 1677 | C   | THR | A | 232 | 38.357 | 17.351 | 43.071 | 1.00 | 9.12  | A |
| ATOM | 1678 | O   | THR | A | 232 | 37.869 | 16.747 | 42.118 | 1.00 | 13.13 | A |
| ATOM | 1679 | N   | GLY | A | 233 | 38.240 | 16.934 | 44.332 | 1.00 | 9.55  | A |
| ATOM | 1680 | CA  | GLY | A | 233 | 37.466 | 15.739 | 44.636 | 1.00 | 13.57 | A |
| ATOM | 1681 | C   | GLY | A | 233 | 38.197 | 14.616 | 45.364 | 1.00 | 14.09 | A |
| ATOM | 1682 | O   | GLY | A | 233 | 37.634 | 13.556 | 45.591 | 1.00 | 16.30 | A |
| ATOM | 1683 | N   | LYS | A | 234 | 39.460 | 14.831 | 45.706 | 1.00 | 14.67 | A |
| ATOM | 1684 | CA  | LYS | A | 234 | 40.226 | 13.834 | 46.438 | 1.00 | 15.04 | A |
| ATOM | 1685 | CB  | LYS | A | 234 | 41.577 | 14.442 | 46.830 | 1.00 | 13.37 | A |
| ATOM | 1686 | CG  | LYS | A | 234 | 42.483 | 13.576 | 47.688 | 1.00 | 14.40 | A |
| ATOM | 1687 | CD  | LYS | A | 234 | 43.807 | 14.314 | 47.968 | 1.00 | 17.84 | A |
| ATOM | 1688 | CE  | LYS | A | 234 | 43.594 | 15.567 | 48.839 | 1.00 | 15.78 | A |
| ATOM | 1689 | NZ  | LYS | A | 234 | 44.766 | 16.501 | 48.832 | 1.00 | 12.74 | A |
| ATOM | 1690 | C   | LYS | A | 234 | 39.450 | 13.411 | 47.697 | 1.00 | 17.96 | A |
| ATOM | 1691 | O   | LYS | A | 234 | 38.826 | 14.240 | 48.369 | 1.00 | 13.45 | A |
| ATOM | 1692 | N   | GLY | A | 235 | 39.489 | 12.124 | 48.031 | 1.00 | 15.80 | A |
| ATOM | 1693 | CA  | GLY | A | 235 | 38.785 | 11.694 | 49.223 | 1.00 | 15.51 | A |
| ATOM | 1694 | C   | GLY | A | 235 | 38.764 | 10.191 | 49.402 | 1.00 | 19.91 | A |
| ATOM | 1695 | O   | GLY | A | 235 | 39.586 | 9.472  | 48.825 | 1.00 | 21.77 | A |
| ATOM | 1696 | N   | SER | A | 236 | 37.811 | 9.731  | 50.204 | 1.00 | 21.18 | A |
| ATOM | 1697 | CA  | SER | A | 236 | 37.624 | 8.311  | 50.489 | 1.00 | 24.63 | A |
| ATOM | 1698 | CB  | SER | A | 236 | 38.018 | 8.004  | 51.929 | 1.00 | 25.33 | A |
| ATOM | 1699 | OG  | SER | A | 236 | 39.359 | 8.397  | 52.161 | 1.00 | 33.33 | A |
| ATOM | 1700 | C   | SER | A | 236 | 36.159 | 7.969  | 50.291 | 1.00 | 26.45 | A |
| ATOM | 1701 | O   | SER | A | 236 | 35.282 | 8.624  | 50.855 | 1.00 | 27.89 | A |
| ATOM | 1702 | N   | SER | A | 237 | 35.891 | 6.947  | 49.488 | 1.00 | 22.58 | A |
| ATOM | 1703 | CA  | SER | A | 237 | 34.522 | 6.520  | 49.238 | 1.00 | 23.79 | A |
| ATOM | 1704 | CB  | SER | A | 237 | 34.123 | 6.799  | 47.786 | 1.00 | 25.37 | A |
| ATOM | 1705 | OG  | SER | A | 237 | 34.019 | 8.197  | 47.578 | 1.00 | 38.24 | A |
| ATOM | 1706 | C   | SER | A | 237 | 34.429 | 5.036  | 49.514 | 1.00 | 21.92 | A |
| ATOM | 1707 | O   | SER | A | 237 | 35.244 | 4.267  | 49.009 | 1.00 | 20.25 | A |
| ATOM | 1708 | N   | SER | A | 238 | 33.423 | 4.640  | 50.295 | 1.00 | 25.14 | A |
| ATOM | 1709 | CA  | SER | A | 238 | 33.233 | 3.236  | 50.662 | 1.00 | 24.45 | A |
| ATOM | 1710 | CB  | SER | A | 238 | 32.716 | 2.427  | 49.471 | 1.00 | 27.22 | A |
| ATOM | 1711 | OG  | SER | A | 238 | 31.371 | 2.785  | 49.163 | 1.00 | 39.35 | A |
| ATOM | 1712 | C   | SER | A | 238 | 34.559 | 2.670  | 51.159 | 1.00 | 23.39 | A |
| ATOM | 1713 | O   | SER | A | 238 | 34.961 | 1.557  | 50.809 | 1.00 | 24.29 | A |
| ATOM | 1714 | N   | GLY | A | 239 | 35.249 | 3.468  | 51.966 | 1.00 | 24.50 | A |
| ATOM | 1715 | CA  | GLY | A | 239 | 36.519 | 3.040  | 52.524 | 1.00 | 25.11 | A |
| ATOM | 1716 | C   | GLY | A | 239 | 37.705 | 2.973  | 51.584 | 1.00 | 28.40 | A |
| ATOM | 1717 | O   | GLY | A | 239 | 38.755 | 2.452  | 51.969 | 1.00 | 28.03 | A |
| ATOM | 1718 | N   | GLY | A | 240 | 37.563 | 3.495  | 50.365 | 1.00 | 21.59 | A |
| ATOM | 1719 | CA  | GLY | A | 240 | 38.677 | 3.459  | 49.431 | 1.00 | 26.05 | A |
| ATOM | 1720 | C   | GLY | A | 240 | 39.082 | 4.858  | 48.984 | 1.00 | 24.32 | A |
| ATOM | 1721 | O   | GLY | A | 240 | 38.218 | 5.685  | 48.714 | 1.00 | 23.70 | A |
| ATOM | 1722 | N   | GLY | A | 241 | 40.386 | 5.121  | 48.920 | 1.00 | 21.49 | A |
| ATOM | 1723 | CA  | GLY | A | 241 | 40.873 | 6.422  | 48.500 | 1.00 | 27.38 | A |
| ATOM | 1724 | C   | GLY | A | 241 | 40.495 | 6.715  | 47.058 | 1.00 | 28.81 | A |
| ATOM | 1725 | O   | GLY | A | 241 | 40.585 | 5.840  | 46.200 | 1.00 | 28.58 | A |
| ATOM | 1726 | N   | ALA | A | 242 | 40.057 | 7.939  | 46.784 | 1.00 | 24.66 | A |
| ATOM | 1727 | CA  | ALA | A | 242 | 39.663 | 8.303  | 45.434 | 1.00 | 22.08 | A |
| ATOM | 1728 | CB  | ALA | A | 242 | 38.159 | 8.527  | 45.367 | 1.00 | 25.95 | A |
| ATOM | 1729 | C   | ALA | A | 242 | 40.385 | 9.573  | 45.043 | 1.00 | 22.46 | A |
| ATOM | 1730 | O   | ALA | A | 242 | 40.541 | 10.472 | 45.869 | 1.00 | 16.67 | A |
| ATOM | 1731 | N   | GLU | A | 243 | 40.813 | 9.647  | 43.785 | 1.00 | 16.24 | A |
| ATOM | 1732 | CA  | GLU | A | 243 | 41.502 | 10.830 | 43.289 | 1.00 | 18.78 | A |
| ATOM | 1733 | CB  | GLU | A | 243 | 42.444 | 10.473 | 42.132 | 1.00 | 23.30 | A |
| ATOM | 1734 | CG  | GLU | A | 243 | 43.643 | 9.624  | 42.499 | 1.00 | 31.37 | A |
| ATOM | 1735 | CD  | GLU | A | 243 | 44.658 | 9.584  | 41.368 | 1.00 | 37.64 | A |
| ATOM | 1736 | OE1 | GLU | A | 243 | 44.234 | 9.507  | 40.195 | 1.00 | 38.59 | A |
| ATOM | 1737 | OE2 | GLU | A | 243 | 45.876 | 9.628  | 41.644 | 1.00 | 41.94 | A |
| ATOM | 1738 | C   | GLU | A | 243 | 40.469 | 11.817 | 42.757 | 1.00 | 15.80 | A |
| ATOM | 1739 | O   | GLU | A | 243 | 39.417 | 11.406 | 42.285 | 1.00 | 17.65 | A |
| ATOM | 1740 | N   | GLY | A | 244 | 40.765 | 13.111 | 42.827 | 1.00 | 15.34 | A |
| ATOM | 1741 | CA  | GLY | A | 244 | 39.832 | 14.101 | 42.286 | 1.00 | 16.23 | A |
| ATOM | 1742 | C   | GLY | A | 244 | 39.994 | 14.161 | 40.770 | 1.00 | 16.48 | A |
| ATOM | 1743 | O   | GLY | A | 244 | 40.894 | 13.528 | 40.228 | 1.00 | 14.37 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1744 | N   | LYS | A | 245 | 39.148 | 14.939 | 40.096 | 1.00 | 14.99 | A |
| ATOM | 1745 | CA  | LYS | A | 245 | 39.186 | 15.079 | 38.632 | 1.00 | 14.88 | A |
| ATOM | 1746 | CB  | LYS | A | 245 | 37.792 | 14.795 | 38.060 | 1.00 | 13.06 | A |
| ATOM | 1747 | CG  | LYS | A | 245 | 37.294 | 13.363 | 38.289 | 1.00 | 22.95 | A |
| ATOM | 1748 | CD  | LYS | A | 245 | 38.174 | 12.353 | 37.540 | 1.00 | 27.44 | A |
| ATOM | 1749 | CE  | LYS | A | 245 | 37.596 | 10.939 | 37.643 | 1.00 | 27.64 | A |
| ATOM | 1750 | NZ  | LYS | A | 245 | 37.298 | 10.599 | 39.063 | 1.00 | 36.34 | A |
| ATOM | 1751 | C   | LYS | A | 245 | 39.617 | 16.471 | 38.165 | 1.00 | 13.81 | A |
| ATOM | 1752 | O   | LYS | A | 245 | 39.580 | 17.431 | 38.932 | 1.00 | 10.66 | A |
| ATOM | 1753 | N   | SER | A | 246 | 40.022 | 16.572 | 36.902 | 1.00 | 14.72 | A |
| ATOM | 1754 | CA  | SER | A | 246 | 40.405 | 17.856 | 36.344 | 1.00 | 11.87 | A |
| ATOM | 1755 | CB  | SER | A | 246 | 41.299 | 17.687 | 35.104 | 1.00 | 12.31 | A |
| ATOM | 1756 | OG  | SER | A | 246 | 40.515 | 17.215 | 34.011 | 1.00 | 9.67  | A |
| ATOM | 1757 | C   | SER | A | 246 | 39.095 | 18.500 | 35.913 | 1.00 | 10.79 | A |
| ATOM | 1758 | O   | SER | A | 246 | 38.076 | 17.815 | 35.735 | 1.00 | 10.08 | A |
| ATOM | 1759 | N   | PRO | A | 247 | 39.114 | 19.825 | 35.698 | 1.00 | 10.98 | A |
| ATOM | 1760 | CD  | PRO | A | 247 | 40.243 | 20.747 | 35.947 | 1.00 | 7.03  | A |
| ATOM | 1761 | CA  | PRO | A | 247 | 37.909 | 20.545 | 35.275 | 1.00 | 9.29  | A |
| ATOM | 1762 | CB  | PRO | A | 247 | 38.210 | 21.988 | 35.692 | 1.00 | 7.19  | A |
| ATOM | 1763 | CG  | PRO | A | 247 | 39.737 | 22.094 | 35.385 | 1.00 | 9.12  | A |
| ATOM | 1764 | C   | PRO | A | 247 | 37.632 | 20.416 | 33.765 | 1.00 | 9.99  | A |
| ATOM | 1765 | O   | PRO | A | 247 | 36.865 | 21.197 | 33.222 | 1.00 | 11.54 | A |
| ATOM | 1766 | N   | ALA | A | 248 | 38.253 | 19.449 | 33.083 | 1.00 | 9.23  | A |
| ATOM | 1767 | CA  | ALA | A | 248 | 37.992 | 19.278 | 31.638 | 1.00 | 12.63 | A |
| ATOM | 1768 | CB  | ALA | A | 248 | 38.832 | 18.097 | 31.069 | 1.00 | 10.35 | A |
| ATOM | 1769 | C   | ALA | A | 248 | 36.487 | 19.021 | 31.431 | 1.00 | 15.07 | A |
| ATOM | 1770 | O   | ALA | A | 248 | 35.838 | 18.390 | 32.278 | 1.00 | 11.60 | A |
| ATOM | 1771 | N   | ALA | A | 249 | 35.935 | 19.497 | 30.311 | 1.00 | 12.95 | A |
| ATOM | 1772 | CA  | ALA | A | 249 | 34.498 | 19.332 | 30.037 | 1.00 | 11.90 | A |
| ATOM | 1773 | CB  | ALA | A | 249 | 34.141 | 19.886 | 28.633 | 1.00 | 12.61 | A |
| ATOM | 1774 | C   | ALA | A | 249 | 34.037 | 17.890 | 30.149 | 1.00 | 15.30 | A |
| ATOM | 1775 | O   | ALA | A | 249 | 32.953 | 17.617 | 30.666 | 1.00 | 14.63 | A |
| ATOM | 1776 | N   | ALA | A | 250 | 34.845 | 16.949 | 29.672 | 1.00 | 14.76 | A |
| ATOM | 1777 | CA  | ALA | A | 250 | 34.426 | 15.542 | 29.769 | 1.00 | 18.41 | A |
| ATOM | 1778 | CB  | ALA | A | 250 | 35.486 | 14.623 | 29.168 | 1.00 | 15.53 | A |
| ATOM | 1779 | C   | ALA | A | 250 | 34.118 | 15.102 | 31.200 | 1.00 | 15.76 | A |
| ATOM | 1780 | O   | ALA | A | 250 | 33.366 | 14.154 | 31.410 | 1.00 | 14.59 | A |
| ATOM | 1781 | N   | ASN | A | 251 | 34.677 | 15.785 | 32.190 | 1.00 | 14.82 | A |
| ATOM | 1782 | CA  | ASN | A | 251 | 34.433 | 15.380 | 33.575 | 1.00 | 13.85 | A |
| ATOM | 1783 | CB  | ASN | A | 251 | 35.665 | 15.696 | 34.441 | 1.00 | 12.26 | A |
| ATOM | 1784 | CG  | ASN | A | 251 | 36.880 | 14.885 | 34.022 | 1.00 | 14.85 | A |
| ATOM | 1785 | OD1 | ASN | A | 251 | 36.755 | 13.712 | 33.653 | 1.00 | 14.23 | A |
| ATOM | 1786 | ND2 | ASN | A | 251 | 38.056 | 15.487 | 34.091 | 1.00 | 13.09 | A |
| ATOM | 1787 | C   | ASN | A | 251 | 33.168 | 15.968 | 34.210 | 1.00 | 16.10 | A |
| ATOM | 1788 | O   | ASN | A | 251 | 32.877 | 15.686 | 35.357 | 1.00 | 14.41 | A |
| ATOM | 1789 | N   | SER | A | 252 | 32.431 | 16.806 | 33.482 | 1.00 | 13.25 | A |
| ATOM | 1790 | CA  | SER | A | 252 | 31.191 | 17.346 | 34.039 | 1.00 | 10.81 | A |
| ATOM | 1791 | CB  | SER | A | 252 | 31.262 | 18.868 | 34.209 | 1.00 | 22.32 | A |
| ATOM | 1792 | OG  | SER | A | 252 | 31.266 | 19.536 | 32.953 | 1.00 | 23.58 | A |
| ATOM | 1793 | C   | SER | A | 252 | 30.027 | 16.982 | 33.101 | 1.00 | 11.68 | A |
| ATOM | 1794 | O   | SER | A | 252 | 28.862 | 17.077 | 33.479 | 1.00 | 12.18 | A |
| ATOM | 1795 | N   | SER | A | 253 | 30.365 | 16.501 | 31.904 | 1.00 | 11.74 | A |
| ATOM | 1796 | CA  | SER | A | 253 | 29.367 | 16.138 | 30.918 | 1.00 | 10.64 | A |
| ATOM | 1797 | CB  | SER | A | 253 | 30.048 | 15.572 | 29.665 | 1.00 | 18.81 | A |
| ATOM | 1798 | OG  | SER | A | 253 | 29.052 | 15.263 | 28.704 | 1.00 | 27.87 | A |
| ATOM | 1799 | C   | SER | A | 253 | 28.294 | 15.139 | 31.382 | 1.00 | 15.51 | A |
| ATOM | 1800 | O   | SER | A | 253 | 27.112 | 15.319 | 31.102 | 1.00 | 11.29 | A |
| ATOM | 1801 | N   | ALA | A | 254 | 28.692 | 14.080 | 32.081 | 1.00 | 12.85 | A |
| ATOM | 1802 | CA  | ALA | A | 254 | 27.700 | 13.084 | 32.525 | 1.00 | 14.75 | A |
| ATOM | 1803 | CB  | ALA | A | 254 | 28.423 | 11.868 | 33.216 | 1.00 | 13.94 | A |
| ATOM | 1804 | C   | ALA | A | 254 | 26.656 | 13.667 | 33.472 | 1.00 | 14.13 | A |
| ATOM | 1805 | O   | ALA | A | 254 | 25.457 | 13.394 | 33.342 | 1.00 | 14.40 | A |
| ATOM | 1806 | N   | ALA | A | 255 | 27.111 | 14.457 | 34.441 | 1.00 | 11.77 | A |
| ATOM | 1807 | CA  | ALA | A | 255 | 26.205 | 15.070 | 35.401 | 1.00 | 13.30 | A |
| ATOM | 1808 | CB  | ALA | A | 255 | 27.009 | 15.838 | 36.460 | 1.00 | 12.60 | A |
| ATOM | 1809 | C   | ALA | A | 255 | 25.223 | 16.017 | 34.698 | 1.00 | 15.34 | A |
| ATOM | 1810 | O   | ALA | A | 255 | 24.068 | 16.162 | 35.113 | 1.00 | 14.03 | A |
| ATOM | 1811 | N   | ILE | A | 256 | 25.684 | 16.680 | 33.644 | 1.00 | 13.10 | A |
| ATOM | 1812 | CA  | ILE | A | 256 | 24.812 | 17.599 | 32.920 | 1.00 | 14.09 | A |
| ATOM | 1813 | CB  | ILE | A | 256 | 25.614 | 18.445 | 31.900 | 1.00 | 11.60 | A |
| ATOM | 1814 | CG2 | ILE | A | 256 | 24.655 | 19.233 | 30.987 | 1.00 | 13.12 | A |
| ATOM | 1815 | CG1 | ILE | A | 256 | 26.577 | 19.378 | 32.657 | 1.00 | 8.87  | A |
| ATOM | 1816 | CD1 | ILE | A | 256 | 25.878 | 20.335 | 33.703 | 1.00 | 6.00  | A |
| ATOM | 1817 | C   | ILE | A | 256 | 23.716 | 16.813 | 32.195 | 1.00 | 12.88 | A |
| ATOM | 1818 | O   | ILE | A | 256 | 22.569 | 17.268 | 32.118 | 1.00 | 12.14 | A |
| ATOM | 1819 | N   | SER | A | 257 | 24.069 | 15.639 | 31.678 | 1.00 | 12.01 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1820 | CA  | SER | A | 257 | 23.105 | 14.793 | 30.960 | 1.00 | 17.17 | A |
| ATOM | 1821 | CB  | SER | A | 257 | 23.773 | 13.529 | 30.418 | 1.00 | 20.37 | A |
| ATOM | 1822 | OG  | SER | A | 257 | 24.331 | 13.802 | 29.157 | 1.00 | 27.40 | A |
| ATOM | 1823 | C   | SER | A | 257 | 21.886 | 14.359 | 31.750 | 1.00 | 21.46 | A |
| ATOM | 1824 | O   | SER | A | 257 | 20.885 | 13.975 | 31.161 | 1.00 | 25.54 | A |
| ATOM | 1825 | N   | VAL | A | 258 | 21.949 | 14.417 | 33.070 | 1.00 | 18.37 | A |
| ATOM | 1826 | CA  | VAL | A | 258 | 20.803 | 13.983 | 33.849 | 1.00 | 22.61 | A |
| ATOM | 1827 | CB  | VAL | A | 258 | 21.230 | 13.049 | 34.996 | 1.00 | 23.45 | A |
| ATOM | 1828 | CG1 | VAL | A | 258 | 22.055 | 11.887 | 34.443 | 1.00 | 28.56 | A |
| ATOM | 1829 | CG2 | VAL | A | 258 | 22.004 | 13.831 | 36.041 | 1.00 | 29.85 | A |
| ATOM | 1830 | C   | VAL | A | 258 | 20.002 | 15.133 | 34.436 | 1.00 | 20.13 | A |
| ATOM | 1831 | O   | VAL | A | 258 | 19.056 | 14.907 | 35.193 | 1.00 | 19.13 | A |
| ATOM | 1832 | N   | VAL | A | 259 | 20.367 | 16.365 | 34.092 | 1.00 | 17.82 | A |
| ATOM | 1833 | CA  | VAL | A | 259 | 19.628 | 17.503 | 34.621 | 1.00 | 12.10 | A |
| ATOM | 1834 | CB  | VAL | A | 259 | 20.345 | 18.816 | 34.305 | 1.00 | 9.61  | A |
| ATOM | 1835 | CG1 | VAL | A | 259 | 19.448 | 20.009 | 34.655 | 1.00 | 9.95  | A |
| ATOM | 1836 | CG2 | VAL | A | 259 | 21.661 | 18.870 | 35.110 | 1.00 | 9.60  | A |
| ATOM | 1837 | C   | VAL | A | 259 | 18.257 | 17.470 | 33.946 | 1.00 | 10.93 | A |
| ATOM | 1838 | O   | VAL | A | 259 | 18.154 | 17.543 | 32.719 | 1.00 | 12.34 | A |
| ATOM | 1839 | N   | PRO | A | 260 | 17.185 | 17.372 | 34.746 | 1.00 | 12.49 | A |
| ATOM | 1840 | CD  | PRO | A | 260 | 17.178 | 17.349 | 36.227 | 1.00 | 15.54 | A |
| ATOM | 1841 | CA  | PRO | A | 260 | 15.823 | 17.321 | 34.204 | 1.00 | 12.14 | A |
| ATOM | 1842 | CB  | PRO | A | 260 | 14.992 | 16.881 | 35.415 | 1.00 | 18.68 | A |
| ATOM | 1843 | CG  | PRO | A | 260 | 15.705 | 17.553 | 36.556 | 1.00 | 20.90 | A |
| ATOM | 1844 | C   | PRO | A | 260 | 15.326 | 18.629 | 33.592 | 1.00 | 13.33 | A |
| ATOM | 1845 | O   | PRO | A | 260 | 15.719 | 19.704 | 34.025 | 1.00 | 11.59 | A |
| ATOM | 1846 | N   | LEU | A | 261 | 14.462 | 18.517 | 32.583 | 1.00 | 10.89 | A |
| ATOM | 1847 | CA  | LEU | A | 261 | 13.906 | 19.697 | 31.899 | 1.00 | 14.89 | A |
| ATOM | 1848 | CB  | LEU | A | 261 | 13.190 | 19.272 | 30.612 | 1.00 | 14.36 | A |
| ATOM | 1849 | CG  | LEU | A | 261 | 14.033 | 18.724 | 29.470 | 1.00 | 23.33 | A |
| ATOM | 1850 | CD1 | LEU | A | 261 | 13.132 | 18.115 | 28.388 | 1.00 | 17.91 | A |
| ATOM | 1851 | CD2 | LEU | A | 261 | 14.860 | 19.854 | 28.927 | 1.00 | 21.86 | A |
| ATOM | 1852 | C   | LEU | A | 261 | 12.868 | 20.354 | 32.782 | 1.00 | 14.14 | A |
| ATOM | 1853 | O   | LEU | A | 261 | 12.313 | 19.715 | 33.667 | 1.00 | 13.00 | A |
| ATOM | 1854 | N   | PRO | A | 262 | 12.598 | 21.646 | 32.570 | 1.00 | 16.56 | A |
| ATOM | 1855 | CD  | PRO | A | 262 | 13.154 | 22.620 | 31.613 | 1.00 | 18.10 | A |
| ATOM | 1856 | CA  | PRO | A | 262 | 11.576 | 22.260 | 33.421 | 1.00 | 16.86 | A |
| ATOM | 1857 | CB  | PRO | A | 262 | 11.753 | 23.752 | 33.137 | 1.00 | 16.37 | A |
| ATOM | 1858 | CG  | PRO | A | 262 | 12.147 | 23.764 | 31.698 | 1.00 | 22.55 | A |
| ATOM | 1859 | C   | PRO | A | 262 | 10.239 | 21.709 | 32.911 | 1.00 | 14.68 | A |
| ATOM | 1860 | O   | PRO | A | 262 | 10.136 | 21.357 | 31.743 | 1.00 | 14.32 | A |
| ATOM | 1861 | N   | ALA | A | 263 | 9.234  | 21.605 | 33.776 | 1.00 | 13.42 | A |
| ATOM | 1862 | CA  | ALA | A | 263 | 7.943  | 21.085 | 33.344 | 1.00 | 16.60 | A |
| ATOM | 1863 | CB  | ALA | A | 263 | 6.994  | 20.952 | 34.539 | 1.00 | 20.02 | A |
| ATOM | 1864 | C   | ALA | A | 263 | 7.343  | 22.011 | 32.292 | 1.00 | 16.04 | A |
| ATOM | 1865 | O   | ALA | A | 263 | 7.480  | 23.235 | 32.377 | 1.00 | 14.70 | A |
| ATOM | 1866 | N   | ALA | A | 264 | 6.664  | 21.426 | 31.309 | 1.00 | 15.42 | A |
| ATOM | 1867 | CA  | ALA | A | 264 | 6.050  | 22.206 | 30.239 | 1.00 | 12.74 | A |
| ATOM | 1868 | CB  | ALA | A | 264 | 5.248  | 21.287 | 29.308 | 1.00 | 19.88 | A |
| ATOM | 1869 | C   | ALA | A | 264 | 5.149  | 23.329 | 30.747 | 1.00 | 15.82 | A |
| ATOM | 1870 | O   | ALA | A | 264 | 5.247  | 24.461 | 30.264 | 1.00 | 17.34 | A |
| ATOM | 1871 | N   | ALA | A | 265 | 4.284  | 23.037 | 31.721 | 1.00 | 13.78 | A |
| ATOM | 1872 | CA  | ALA | A | 265 | 3.370  | 24.071 | 32.242 | 1.00 | 15.17 | A |
| ATOM | 1873 | CB  | ALA | A | 265 | 2.464  | 23.478 | 33.363 | 1.00 | 15.42 | A |
| ATOM | 1874 | C   | ALA | A | 265 | 4.057  | 25.333 | 32.772 | 1.00 | 15.06 | A |
| ATOM | 1875 | O   | ALA | A | 265 | 3.437  | 26.398 | 32.838 | 1.00 | 13.78 | A |
| ATOM | 1876 | N   | ASN | A | 266 | 5.320  | 25.212 | 33.175 | 1.00 | 13.85 | A |
| ATOM | 1877 | CA  | ASN | A | 266 | 6.057  | 26.343 | 33.733 | 1.00 | 12.11 | A |
| ATOM | 1878 | CB  | ASN | A | 266 | 6.987  | 25.895 | 34.873 | 1.00 | 13.94 | A |
| ATOM | 1879 | CG  | ASN | A | 266 | 6.253  | 25.239 | 36.028 | 1.00 | 23.25 | A |
| ATOM | 1880 | OD1 | ASN | A | 266 | 5.175  | 25.676 | 36.425 | 1.00 | 21.92 | A |
| ATOM | 1881 | ND2 | ASN | A | 266 | 6.856  | 24.200 | 36.592 | 1.00 | 19.37 | A |
| ATOM | 1882 | C   | ASN | A | 266 | 6.969  | 27.039 | 32.730 | 1.00 | 12.06 | A |
| ATOM | 1883 | O   | ASN | A | 266 | 7.662  | 27.965 | 33.100 | 1.00 | 13.88 | A |
| ATOM | 1884 | N   | ARG | A | 267 | 6.980  | 26.600 | 31.483 | 1.00 | 10.11 | A |
| ATOM | 1885 | CA  | ARG | A | 267 | 7.933  | 27.162 | 30.534 | 1.00 | 12.44 | A |
| ATOM | 1886 | CB  | ARG | A | 267 | 8.029  | 26.254 | 29.306 | 1.00 | 10.57 | A |
| ATOM | 1887 | CG  | ARG | A | 267 | 8.746  | 24.945 | 29.675 | 1.00 | 12.04 | A |
| ATOM | 1888 | CD  | ARG | A | 267 | 8.892  | 23.924 | 28.540 | 1.00 | 9.95  | A |
| ATOM | 1889 | NE  | ARG | A | 267 | 9.275  | 22.637 | 29.124 | 1.00 | 14.76 | A |
| ATOM | 1890 | CZ  | ARG | A | 267 | 9.533  | 21.530 | 28.439 | 1.00 | 14.94 | A |
| ATOM | 1891 | NH1 | ARG | A | 267 | 9.477  | 21.543 | 27.118 | 1.00 | 16.59 | A |
| ATOM | 1892 | NH2 | ARG | A | 267 | 9.782  | 20.387 | 29.084 | 1.00 | 12.17 | A |
| ATOM | 1893 | C   | ARG | A | 267 | 7.785  | 28.629 | 30.168 | 1.00 | 13.15 | A |
| ATOM | 1894 | O   | ARG | A | 267 | 8.658  | 29.207 | 29.505 | 1.00 | 13.32 | A |
| ATOM | 1895 | N   | GLY | A | 268 | 6.711  | 29.240 | 30.663 | 1.00 | 11.13 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1896 | CA  | GLY | A | 268 | 6.491  | 30.653 | 30.439 | 1.00 | 13.33 | A |
| ATOM | 1897 | C   | GLY | A | 268 | 7.212  | 31.457 | 31.507 | 1.00 | 13.92 | A |
| ATOM | 1898 | O   | GLY | A | 268 | 7.219  | 32.679 | 31.452 | 1.00 | 14.39 | A |
| ATOM | 1899 | N   | ASP | A | 269 | 7.804  | 30.767 | 32.486 | 1.00 | 11.00 | A |
| ATOM | 1900 | CA  | ASP | A | 269 | 8.554  | 31.398 | 33.594 | 1.00 | 14.58 | A |
| ATOM | 1901 | CB  | ASP | A | 269 | 8.233  | 30.665 | 34.914 | 1.00 | 13.17 | A |
| ATOM | 1902 | CG  | ASP | A | 269 | 8.943  | 31.263 | 36.117 | 1.00 | 16.24 | A |
| ATOM | 1903 | OD1 | ASP | A | 269 | 9.767  | 32.179 | 35.944 | 1.00 | 17.40 | A |
| ATOM | 1904 | OD2 | ASP | A | 269 | 8.667  | 30.804 | 37.244 | 1.00 | 19.44 | A |
| ATOM | 1905 | C   | ASP | A | 269 | 10.064 | 31.290 | 33.303 | 1.00 | 10.72 | A |
| ATOM | 1906 | O   | ASP | A | 269 | 10.616 | 30.196 | 33.348 | 1.00 | 11.39 | A |
| ATOM | 1907 | N   | PRO | A | 270 | 10.742 | 32.417 | 33.010 | 1.00 | 11.52 | A |
| ATOM | 1908 | CD  | PRO | A | 270 | 10.217 | 33.796 | 32.924 | 1.00 | 11.48 | A |
| ATOM | 1909 | CA  | PRO | A | 270 | 12.184 | 32.394 | 32.709 | 1.00 | 10.44 | A |
| ATOM | 1910 | CB  | PRO | A | 270 | 12.523 | 33.867 | 32.491 | 1.00 | 11.04 | A |
| ATOM | 1911 | CG  | PRO | A | 270 | 11.225 | 34.465 | 32.026 | 1.00 | 13.30 | A |
| ATOM | 1912 | C   | PRO | A | 270 | 13.042 | 31.786 | 33.793 | 1.00 | 12.77 | A |
| ATOM | 1913 | O   | PRO | A | 270 | 14.097 | 31.243 | 33.521 | 1.00 | 10.58 | A |
| ATOM | 1914 | N   | ASN | A | 271 | 12.578 | 31.870 | 35.032 | 1.00 | 11.41 | A |
| ATOM | 1915 | CA  | ASN | A | 271 | 13.337 | 31.332 | 36.145 | 1.00 | 11.19 | A |
| ATOM | 1916 | CB  | ASN | A | 271 | 12.660 | 31.729 | 37.463 | 1.00 | 14.43 | A |
| ATOM | 1917 | CG  | ASN | A | 271 | 13.533 | 31.434 | 38.683 | 1.00 | 22.14 | A |
| ATOM | 1918 | OD1 | ASN | A | 271 | 14.734 | 31.726 | 38.696 | 1.00 | 16.89 | A |
| ATOM | 1919 | ND2 | ASN | A | 271 | 12.934 | 30.854 | 39.703 | 1.00 | 16.43 | A |
| ATOM | 1920 | C   | ASN | A | 271 | 13.545 | 29.816 | 36.090 | 1.00 | 16.21 | A |
| ATOM | 1921 | O   | ASN | A | 271 | 14.595 | 29.319 | 36.510 | 1.00 | 15.74 | A |
| ATOM | 1922 | N   | VAL | A | 272 | 12.574 | 29.065 | 35.575 | 1.00 | 10.21 | A |
| ATOM | 1923 | CA  | VAL | A | 272 | 12.749 | 27.613 | 35.547 | 1.00 | 11.32 | A |
| ATOM | 1924 | CB  | VAL | A | 272 | 11.378 | 26.849 | 35.440 | 1.00 | 13.38 | A |
| ATOM | 1925 | CG1 | VAL | A | 272 | 10.450 | 27.297 | 36.548 | 1.00 | 14.31 | A |
| ATOM | 1926 | CG2 | VAL | A | 272 | 10.759 | 27.074 | 34.078 | 1.00 | 11.03 | A |
| ATOM | 1927 | C   | VAL | A | 272 | 13.651 | 27.086 | 34.434 | 1.00 | 12.71 | A |
| ATOM | 1928 | O   | VAL | A | 272 | 14.028 | 25.907 | 34.459 | 1.00 | 10.89 | A |
| ATOM | 1929 | N   | TRP | A | 273 | 13.991 | 27.930 | 33.461 | 1.00 | 7.57  | A |
| ATOM | 1930 | CA  | TRP | A | 273 | 14.862 | 27.465 | 32.366 | 1.00 | 7.83  | A |
| ATOM | 1931 | CB  | TRP | A | 273 | 14.741 | 28.403 | 31.150 | 1.00 | 7.08  | A |
| ATOM | 1932 | CG  | TRP | A | 273 | 13.496 | 28.126 | 30.364 | 1.00 | 10.87 | A |
| ATOM | 1933 | CD2 | TRP | A | 273 | 13.359 | 27.161 | 29.325 | 1.00 | 9.80  | A |
| ATOM | 1934 | CE2 | TRP | A | 273 | 12.020 | 27.228 | 28.860 | 1.00 | 9.21  | A |
| ATOM | 1935 | CE3 | TRP | A | 273 | 14.241 | 26.240 | 28.732 | 1.00 | 10.74 | A |
| ATOM | 1936 | CD1 | TRP | A | 273 | 12.271 | 28.728 | 30.500 | 1.00 | 7.74  | A |
| ATOM | 1937 | NE1 | TRP | A | 273 | 11.375 | 28.192 | 29.590 | 1.00 | 12.31 | A |
| ATOM | 1938 | CZ2 | TRP | A | 273 | 11.545 | 26.412 | 27.838 | 1.00 | 10.97 | A |
| ATOM | 1939 | CZ3 | TRP | A | 273 | 13.764 | 25.428 | 27.700 | 1.00 | 10.91 | A |
| ATOM | 1940 | CH2 | TRP | A | 273 | 12.427 | 25.522 | 27.267 | 1.00 | 14.13 | A |
| ATOM | 1941 | C   | TRP | A | 273 | 16.338 | 27.311 | 32.755 | 1.00 | 9.26  | A |
| ATOM | 1942 | O   | TRP | A | 273 | 17.119 | 26.663 | 32.042 | 1.00 | 9.73  | A |
| ATOM | 1943 | N   | THR | A | 274 | 16.736 | 27.893 | 33.880 | 1.00 | 8.74  | A |
| ATOM | 1944 | CA  | THR | A | 274 | 18.123 | 27.769 | 34.281 | 1.00 | 11.71 | A |
| ATOM | 1945 | CB  | THR | A | 274 | 18.759 | 29.147 | 34.542 | 1.00 | 12.87 | A |
| ATOM | 1946 | OG1 | THR | A | 274 | 18.701 | 29.940 | 33.334 | 1.00 | 16.61 | A |
| ATOM | 1947 | CG2 | THR | A | 274 | 20.240 | 28.973 | 34.959 | 1.00 | 9.96  | A |
| ATOM | 1948 | C   | THR | A | 274 | 18.271 | 26.918 | 35.535 | 1.00 | 10.53 | A |
| ATOM | 1949 | O   | THR | A | 274 | 18.020 | 27.378 | 36.645 | 1.00 | 11.96 | A |
| ATOM | 1950 | N   | PRO | A | 275 | 18.673 | 25.657 | 35.373 | 1.00 | 11.80 | A |
| ATOM | 1951 | CD  | PRO | A | 275 | 18.885 | 24.916 | 34.119 | 1.00 | 13.30 | A |
| ATOM | 1952 | CA  | PRO | A | 275 | 18.841 | 24.782 | 36.543 | 1.00 | 11.14 | A |
| ATOM | 1953 | CB  | PRO | A | 275 | 19.180 | 23.424 | 35.921 | 1.00 | 15.21 | A |
| ATOM | 1954 | CG  | PRO | A | 275 | 18.600 | 23.506 | 34.528 | 1.00 | 15.39 | A |
| ATOM | 1955 | C   | PRO | A | 275 | 20.004 | 25.253 | 37.445 | 1.00 | 12.51 | A |
| ATOM | 1956 | O   | PRO | A | 275 | 21.007 | 25.723 | 36.950 | 1.00 | 12.15 | A |
| ATOM | 1957 | N   | VAL | A | 276 | 19.869 | 25.148 | 38.764 | 1.00 | 9.91  | A |
| ATOM | 1958 | CA  | VAL | A | 276 | 20.999 | 25.502 | 39.615 | 1.00 | 10.08 | A |
| ATOM | 1959 | CB  | VAL | A | 276 | 20.738 | 26.762 | 40.478 | 1.00 | 15.02 | A |
| ATOM | 1960 | CG1 | VAL | A | 276 | 20.534 | 27.990 | 39.568 | 1.00 | 16.57 | A |
| ATOM | 1961 | CG2 | VAL | A | 276 | 19.551 | 26.543 | 41.388 | 1.00 | 17.45 | A |
| ATOM | 1962 | C   | VAL | A | 276 | 21.236 | 24.293 | 40.500 | 1.00 | 12.75 | A |
| ATOM | 1963 | O   | VAL | A | 276 | 20.315 | 23.498 | 40.743 | 1.00 | 7.21  | A |
| ATOM | 1964 | N   | PHE | A | 277 | 22.472 | 24.149 | 40.969 | 1.00 | 13.38 | A |
| ATOM | 1965 | CA  | PHE | A | 277 | 22.848 | 23.017 | 41.798 | 1.00 | 12.43 | A |
| ATOM | 1966 | CB  | PHE | A | 277 | 24.231 | 22.491 | 41.373 | 1.00 | 8.49  | A |
| ATOM | 1967 | CG  | PHE | A | 277 | 24.229 | 21.828 | 40.017 | 1.00 | 8.19  | A |
| ATOM | 1968 | CD1 | PHE | A | 277 | 24.404 | 22.568 | 38.858 | 1.00 | 9.76  | A |
| ATOM | 1969 | CD2 | PHE | A | 277 | 23.999 | 20.461 | 39.909 | 1.00 | 8.15  | A |
| ATOM | 1970 | CE1 | PHE | A | 277 | 24.350 | 21.934 | 37.585 | 1.00 | 13.41 | A |
| ATOM | 1971 | CE2 | PHE | A | 277 | 23.938 | 19.825 | 38.654 | 1.00 | 13.62 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 1972 | CZ  | PHE | A | 277 | 24.114 | 20.555 | 37.499 | 1.00 | 8.74  | A |
| ATOM | 1973 | C   | PHE | A | 277 | 22.848 | 23.377 | 43.272 | 1.00 | 12.19 | A |
| ATOM | 1974 | O   | PHE | A | 277 | 22.892 | 24.553 | 43.534 | 1.00 | 12.80 | A |
| ATOM | 1975 | N   | GLY | A | 278 | 22.781 | 22.356 | 44.116 | 1.00 | 12.01 | A |
| ATOM | 1976 | CA  | GLY | A | 278 | 22.767 | 22.601 | 45.547 | 1.00 | 10.29 | A |
| ATOM | 1977 | C   | GLY | A | 278 | 23.113 | 21.342 | 46.309 | 1.00 | 9.39  | A |
| ATOM | 1978 | O   | GLY | A | 278 | 23.379 | 20.302 | 45.704 | 1.00 | 12.45 | A |
| ATOM | 1979 | N   | ALA | A | 279 | 23.087 | 21.414 | 47.637 | 1.00 | 11.15 | A |
| ATOM | 1980 | CA  | ALA | A | 279 | 23.436 | 20.246 | 46.450 | 1.00 | 14.32 | A |
| ATOM | 1981 | CB  | ALA | A | 279 | 23.362 | 20.604 | 49.930 | 1.00 | 16.91 | A |
| ATOM | 1982 | C   | ALA | A | 279 | 22.542 | 19.029 | 48.157 | 1.00 | 20.18 | A |
| ATOM | 1983 | O   | ALA | A | 279 | 23.038 | 17.896 | 48.017 | 1.00 | 18.69 | A |
| ATOM | 1984 | N   | VAL | A | 280 | 21.238 | 19.262 | 48.040 | 1.00 | 14.35 | A |
| ATOM | 1985 | CA  | VAL | A | 280 | 20.302 | 18.176 | 47.796 | 1.00 | 19.81 | A |
| ATOM | 1986 | CB  | VAL | A | 280 | 19.500 | 17.847 | 49.076 | 1.00 | 23.28 | A |
| ATOM | 1987 | CG1 | VAL | A | 280 | 20.457 | 17.579 | 50.225 | 1.00 | 23.97 | A |
| ATOM | 1988 | CG2 | VAL | A | 280 | 18.603 | 18.992 | 49.436 | 1.00 | 21.87 | A |
| ATOM | 1989 | C   | VAL | A | 280 | 19.311 | 18.483 | 46.686 | 1.00 | 20.63 | A |
| ATOM | 1990 | O   | VAL | A | 280 | 19.004 | 19.635 | 46.407 | 1.00 | 21.63 | A |
| ATOM | 1991 | N   | THR | A | 281 | 18.812 | 17.436 | 46.055 | 1.00 | 20.03 | A |
| ATOM | 1992 | CA  | THR | A | 281 | 17.838 | 17.599 | 44.982 | 1.00 | 19.32 | A |
| ATOM | 1993 | CB  | THR | A | 281 | 17.732 | 16.327 | 44.136 | 1.00 | 20.70 | A |
| ATOM | 1994 | OG1 | THR | A | 281 | 18.989 | 16.096 | 43.493 | 1.00 | 24.83 | A |
| ATOM | 1995 | CG2 | THR | A | 281 | 16.637 | 16.473 | 43.062 | 1.00 | 20.23 | A |
| ATOM | 1996 | C   | THR | A | 281 | 16.500 | 17.882 | 45.618 | 1.00 | 24.45 | A |
| ATOM | 1997 | O   | THR | A | 281 | 16.073 | 17.159 | 46.520 | 1.00 | 22.56 | A |
| ATOM | 1998 | N   | GLY | A | 282 | 15.854 | 18.949 | 45.164 | 1.00 | 22.37 | A |
| ATOM | 1999 | CA  | GLY | A | 282 | 14.564 | 19.316 | 45.706 | 1.00 | 26.62 | A |
| ATOM | 2000 | C   | GLY | A | 282 | 14.183 | 20.735 | 45.343 | 1.00 | 31.11 | A |
| ATOM | 2001 | O   | GLY | A | 282 | 15.048 | 21.603 | 45.206 | 1.00 | 27.54 | A |
| ATOM | 2002 | N   | GLY | A | 283 | 12.883 | 20.971 | 45.181 | 1.00 | 32.42 | A |
| ATOM | 2003 | CA  | GLY | A | 283 | 12.401 | 22.301 | 44.855 | 1.00 | 30.56 | A |
| ATOM | 2004 | C   | GLY | A | 283 | 13.051 | 22.950 | 43.654 | 1.00 | 30.47 | A |
| ATOM | 2005 | O   | GLY | A | 283 | 13.307 | 24.154 | 43.665 | 1.00 | 33.57 | A |
| ATOM | 2006 | N   | GLY | A | 284 | 13.299 | 22.171 | 42.607 | 1.00 | 26.82 | A |
| ATOM | 2007 | CA  | GLY | A | 284 | 13.925 | 22.723 | 41.415 | 1.00 | 26.01 | A |
| ATOM | 2008 | C   | GLY | A | 284 | 15.450 | 22.687 | 41.439 | 1.00 | 26.04 | A |
| ATOM | 2009 | O   | GLY | A | 284 | 16.115 | 22.822 | 40.406 | 1.00 | 25.82 | A |
| ATOM | 2010 | N   | VAL | A | 285 | 16.022 | 22.521 | 42.622 | 1.00 | 19.46 | A |
| ATOM | 2011 | CA  | VAL | A | 285 | 17.467 | 22.461 | 42.722 | 1.00 | 19.85 | A |
| ATOM | 2012 | CB  | VAL | A | 285 | 17.903 | 22.894 | 44.135 | 1.00 | 19.90 | A |
| ATOM | 2013 | CG1 | VAL | A | 285 | 19.389 | 22.673 | 44.319 | 1.00 | 16.38 | A |
| ATOM | 2014 | CG2 | VAL | A | 285 | 17.521 | 24.376 | 44.360 | 1.00 | 20.29 | A |
| ATOM | 2015 | C   | VAL | A | 285 | 17.958 | 21.037 | 42.428 | 1.00 | 18.72 | A |
| ATOM | 2016 | O   | VAL | A | 285 | 17.298 | 20.055 | 42.754 | 1.00 | 18.51 | A |
| ATOM | 2017 | N   | VAL | A | 286 | 19.103 | 20.932 | 41.755 | 1.00 | 14.01 | A |
| ATOM | 2018 | CA  | VAL | A | 286 | 19.706 | 19.645 | 41.423 | 1.00 | 16.59 | A |
| ATOM | 2019 | CB  | VAL | A | 286 | 20.200 | 19.625 | 39.964 | 1.00 | 14.25 | A |
| ATOM | 2020 | CG1 | VAL | A | 286 | 20.729 | 18.254 | 39.623 | 1.00 | 19.16 | A |
| ATOM | 2021 | CG2 | VAL | A | 286 | 19.058 | 19.997 | 39.036 | 1.00 | 20.67 | A |
| ATOM | 2022 | C   | VAL | A | 286 | 20.917 | 19.416 | 42.325 | 1.00 | 17.27 | A |
| ATOM | 2023 | O   | VAL | A | 286 | 21.757 | 20.302 | 42.484 | 1.00 | 13.49 | A |
| ATOM | 2024 | N   | ALA | A | 287 | 21.041 | 18.229 | 42.896 | 1.00 | 15.01 | A |
| ATOM | 2025 | CA  | ALA | A | 287 | 22.188 | 18.000 | 43.778 | 1.00 | 17.78 | A |
| ATOM | 2026 | CB  | ALA | A | 287 | 22.039 | 16.649 | 44.527 | 1.00 | 16.62 | A |
| ATOM | 2027 | C   | ALA | A | 287 | 23.483 | 18.011 | 42.999 | 1.00 | 12.88 | A |
| ATOM | 2028 | O   | ALA | A | 287 | 23.520 | 17.533 | 41.854 | 1.00 | 10.29 | A |
| ATOM | 2029 | N   | TYR | A | 288 | 24.538 | 18.576 | 43.603 | 1.00 | 11.08 | A |
| ATOM | 2030 | CA  | TYR | A | 288 | 25.867 | 18.554 | 42.979 | 1.00 | 8.88  | A |
| ATOM | 2031 | CB  | TYR | A | 288 | 26.877 | 19.297 | 43.862 | 1.00 | 12.41 | A |
| ATOM | 2032 | CG  | TYR | A | 288 | 26.891 | 20.803 | 43.649 | 1.00 | 9.59  | A |
| ATOM | 2033 | CD1 | TYR | A | 288 | 26.329 | 21.677 | 44.589 | 1.00 | 8.82  | A |
| ATOM | 2034 | CE1 | TYR | A | 288 | 26.320 | 23.086 | 44.382 | 1.00 | 10.11 | A |
| ATOM | 2035 | CD2 | TYR | A | 288 | 27.463 | 21.356 | 42.491 | 1.00 | 10.87 | A |
| ATOM | 2036 | CE2 | TYR | A | 288 | 27.464 | 22.744 | 42.275 | 1.00 | 6.63  | A |
| ATOM | 2037 | CZ  | TYR | A | 288 | 26.883 | 23.601 | 43.223 | 1.00 | 7.60  | A |
| ATOM | 2038 | OH  | TYR | A | 288 | 26.842 | 24.960 | 42.960 | 1.00 | 7.46  | A |
| ATOM | 2039 | C   | TYR | A | 288 | 26.263 | 17.061 | 42.851 | 1.00 | 12.67 | A |
| ATOM | 2040 | O   | TYR | A | 288 | 25.989 | 16.265 | 43.750 | 1.00 | 10.55 | A |
| ATOM | 2041 | N   | PRO | A | 289 | 26.925 | 16.672 | 41.746 | 1.00 | 12.61 | A |
| ATOM | 2042 | CD  | PRO | A | 289 | 27.338 | 17.560 | 40.625 | 1.00 | 13.50 | A |
| ATOM | 2043 | CA  | PRO | A | 289 | 27.346 | 15.280 | 41.495 | 1.00 | 12.99 | A |
| ATOM | 2044 | CB  | PRO | A | 289 | 27.863 | 15.328 | 40.051 | 1.00 | 15.51 | A |
| ATOM | 2045 | CG  | PRO | A | 289 | 28.424 | 16.734 | 39.920 | 1.00 | 10.53 | A |
| ATOM | 2046 | C   | PRO | A | 289 | 28.366 | 14.644 | 42.439 | 1.00 | 17.46 | A |
| ATOM | 2047 | O   | PRO | A | 289 | 29.342 | 15.282 | 42.835 | 1.00 | 15.29 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2048 | N   | ASP | A | 290 | 28.149 | 13.372 | 42.782 | 1.00 | 16.57 | A |
| ATOM | 2049 | CA  | ASP | A | 290 | 29.092 | 12.691 | 43.652 | 1.00 | 20.97 | A |
| ATOM | 2050 | CB  | ASP | A | 290 | 28.360 | 11.751 | 44.628 | 1.00 | 25.52 | A |
| ATOM | 2051 | CG  | ASP | A | 290 | 27.489 | 10.723 | 43.929 | 1.00 | 34.64 | A |
| ATOM | 2052 | OD1 | ASP | A | 290 | 26.599 | 10.146 | 44.604 | 1.00 | 38.07 | A |
| ATOM | 2053 | OD2 | ASP | A | 290 | 27.693 | 10.478 | 42.716 | 1.00 | 39.24 | A |
| ATOM | 2054 | C   | ASP | A | 290 | 30.154 | 11.952 | 42.824 | 1.00 | 21.23 | A |
| ATOM | 2055 | O   | ASP | A | 290 | 30.990 | 11.231 | 43.362 | 1.00 | 21.11 | A |
| ATOM | 2056 | N   | SER | A | 291 | 30.136 | 12.152 | 41.509 | 1.00 | 14.24 | A |
| ATOM | 2057 | CA  | SER | A | 291 | 31.143 | 11.538 | 40.645 | 1.00 | 16.28 | A |
| ATOM | 2058 | CB  | SER | A | 291 | 30.592 | 10.290 | 39.925 | 1.00 | 16.14 | A |
| ATOM | 2059 | OG  | SER | A | 291 | 29.549 | 10.625 | 39.031 | 1.00 | 22.17 | A |
| ATOM | 2060 | C   | SER | A | 291 | 31.555 | 12.609 | 39.643 | 1.00 | 14.75 | A |
| ATOM | 2061 | O   | SER | A | 291 | 30.842 | 13.605 | 39.493 | 1.00 | 13.50 | A |
| ATOM | 2062 | N   | GLY | A | 292 | 32.692 | 12.419 | 38.971 | 1.00 | 13.79 | A |
| ATOM | 2063 | CA  | GLY | A | 292 | 33.181 | 13.423 | 38.019 | 1.00 | 14.60 | A |
| ATOM | 2064 | C   | GLY | A | 292 | 33.713 | 14.688 | 38.707 | 1.00 | 11.05 | A |
| ATOM | 2065 | O   | GLY | A | 292 | 33.964 | 14.669 | 39.909 | 1.00 | 14.10 | A |
| ATOM | 2066 | N   | TYR | A | 293 | 33.904 | 15.779 | 37.955 | 1.00 | 10.56 | A |
| ATOM | 2067 | CA  | TYR | A | 293 | 34.380 | 17.049 | 38.529 | 1.00 | 9.23  | A |
| ATOM | 2068 | CB  | TYR | A | 293 | 34.838 | 18.014 | 37.443 | 1.00 | 10.30 | A |
| ATOM | 2069 | CG  | TYR | A | 293 | 35.535 | 19.229 | 38.012 | 1.00 | 11.13 | A |
| ATOM | 2070 | CD1 | TYR | A | 293 | 36.829 | 19.138 | 38.526 | 1.00 | 7.85  | A |
| ATOM | 2071 | CE1 | TYR | A | 293 | 37.482 | 20.269 | 39.049 | 1.00 | 8.64  | A |
| ATOM | 2072 | CD2 | TYR | A | 293 | 34.900 | 20.470 | 38.038 | 1.00 | 11.82 | A |
| ATOM | 2073 | CE2 | TYR | A | 293 | 35.547 | 21.601 | 38.554 | 1.00 | 11.43 | A |
| ATOM | 2074 | CZ  | TYR | A | 293 | 36.839 | 21.488 | 39.052 | 1.00 | 8.40  | A |
| ATOM | 2075 | OH  | TYR | A | 293 | 37.488 | 22.625 | 39.496 | 1.00 | 8.49  | A |
| ATOM | 2076 | C   | TYR | A | 293 | 33.183 | 17.645 | 39.252 | 1.00 | 9.71  | A |
| ATOM | 2077 | O   | TYR | A | 293 | 32.142 | 17.834 | 38.657 | 1.00 | 12.02 | A |
| ATOM | 2078 | N   | PRO | A | 294 | 33.347 | 18.021 | 40.531 | 1.00 | 12.25 | A |
| ATOM | 2079 | CD  | PRO | A | 294 | 34.575 | 17.923 | 41.350 | 1.00 | 12.44 | A |
| ATOM | 2080 | CA  | PRO | A | 294 | 32.229 | 18.559 | 41.302 | 1.00 | 14.24 | A |
| ATOM | 2081 | CB  | PRO | A | 294 | 32.644 | 18.263 | 42.748 | 1.00 | 12.15 | A |
| ATOM | 2082 | CG  | PRO | A | 294 | 34.132 | 18.499 | 42.712 | 1.00 | 15.49 | A |
| ATOM | 2083 | C   | PRO | A | 294 | 31.682 | 19.963 | 41.133 | 1.00 | 13.85 | A |
| ATOM | 2084 | O   | PRO | A | 294 | 30.511 | 20.171 | 41.429 | 1.00 | 11.37 | A |
| ATOM | 2085 | N   | ILE | A | 295 | 32.476 | 20.907 | 40.628 | 1.00 | 10.88 | A |
| ATOM | 2086 | CA  | ILE | A | 295 | 31.990 | 22.280 | 40.510 | 1.00 | 9.12  | A |
| ATOM | 2087 | CB  | ILE | A | 295 | 33.062 | 23.301 | 40.934 | 1.00 | 10.07 | A |
| ATOM | 2088 | CG2 | ILE | A | 295 | 32.375 | 24.666 | 41.232 | 1.00 | 10.52 | A |
| ATOM | 2089 | CG1 | ILE | A | 295 | 33.733 | 22.853 | 42.236 | 1.00 | 12.06 | A |
| ATOM | 2090 | CD1 | ILE | A | 295 | 34.841 | 23.801 | 42.703 | 1.00 | 12.46 | A |
| ATOM | 2091 | C   | ILE | A | 295 | 31.564 | 22.574 | 39.087 | 1.00 | 12.87 | A |
| ATOM | 2092 | O   | ILE | A | 295 | 32.397 | 22.660 | 38.182 | 1.00 | 10.57 | A |
| ATOM | 2093 | N   | LEU | A | 296 | 30.257 | 22.743 | 38.902 | 1.00 | 10.82 | A |
| ATOM | 2094 | CA  | LEU | A | 296 | 29.703 | 22.951 | 37.570 | 1.00 | 8.61  | A |
| ATOM | 2095 | CB  | LEU | A | 296 | 29.370 | 21.578 | 36.949 | 1.00 | 9.63  | A |
| ATOM | 2096 | CG  | LEU | A | 296 | 28.032 | 20.884 | 37.276 | 1.00 | 7.75  | A |
| ATOM | 2097 | CD1 | LEU | A | 296 | 27.971 | 19.517 | 36.572 | 1.00 | 11.60 | A |
| ATOM | 2098 | CD2 | LEU | A | 296 | 27.852 | 20.690 | 38.784 | 1.00 | 10.20 | A |
| ATOM | 2099 | C   | LEU | A | 296 | 28.461 | 23.828 | 37.612 | 1.00 | 7.00  | A |
| ATOM | 2100 | O   | LEU | A | 296 | 27.945 | 24.137 | 38.690 | 1.00 | 11.47 | A |
| ATOM | 2101 | N   | GLY | A | 297 | 27.988 | 24.236 | 36.436 | 1.00 | 8.98  | A |
| ATOM | 2102 | CA  | GLY | A | 297 | 26.812 | 25.093 | 36.353 | 1.00 | 8.75  | A |
| ATOM | 2103 | C   | GLY | A | 297 | 26.503 | 25.452 | 34.906 | 1.00 | 14.03 | A |
| ATOM | 2104 | O   | GLY | A | 297 | 27.128 | 24.917 | 33.979 | 1.00 | 9.23  | A |
| ATOM | 2105 | N   | PHE | A | 298 | 25.544 | 26.353 | 34.700 | 1.00 | 7.40  | A |
| ATOM | 2106 | CA  | PHE | A | 298 | 25.177 | 26.758 | 33.350 | 1.00 | 7.84  | A |
| ATOM | 2107 | CB  | PHE | A | 298 | 23.666 | 26.550 | 33.105 | 1.00 | 6.30  | A |
| ATOM | 2108 | CG  | PHE | A | 298 | 23.249 | 25.102 | 32.984 | 1.00 | 10.10 | A |
| ATOM | 2109 | CD1 | PHE | A | 298 | 22.775 | 24.398 | 34.094 | 1.00 | 9.62  | A |
| ATOM | 2110 | CD2 | PHE | A | 298 | 23.356 | 24.444 | 31.763 | 1.00 | 8.37  | A |
| ATOM | 2111 | CE1 | PHE | A | 298 | 22.414 | 23.038 | 33.986 | 1.00 | 13.84 | A |
| ATOM | 2112 | CE2 | PHE | A | 298 | 23.005 | 23.087 | 31.630 | 1.00 | 7.19  | A |
| ATOM | 2113 | CZ  | PHE | A | 298 | 22.533 | 22.379 | 32.747 | 1.00 | 12.00 | A |
| ATOM | 2114 | C   | PHE | A | 298 | 25.459 | 28.235 | 33.145 | 1.00 | 10.22 | A |
| ATOM | 2115 | O   | PHE | A | 298 | 25.431 | 29.007 | 34.114 | 1.00 | 9.27  | A |
| ATOM | 2116 | N   | THR | A | 299 | 25.811 | 28.615 | 31.910 | 1.00 | 7.04  | A |
| ATOM | 2117 | CA  | THR | A | 299 | 25.961 | 30.029 | 31.594 | 1.00 | 8.99  | A |
| ATOM | 2118 | CB  | THR | A | 299 | 27.319 | 30.414 | 30.975 | 1.00 | 12.65 | A |
| ATOM | 2119 | OG1 | THR | A | 299 | 27.293 | 31.818 | 30.682 | 1.00 | 10.67 | A |
| ATOM | 2120 | CG2 | THR | A | 299 | 27.616 | 29.617 | 29.740 | 1.00 | 12.18 | A |
| ATOM | 2121 | C   | THR | A | 299 | 24.798 | 30.220 | 30.616 | 1.00 | 8.12  | A |
| ATOM | 2122 | O   | THR | A | 299 | 24.482 | 29.325 | 29.810 | 1.00 | 9.48  | A |
| ATOM | 2123 | N   | ASP | A | 300 | 24.173 | 31.392 | 30.677 | 1.00 | 8.49  | A |

FIGURE 5 (suite)

|      |      |     |       |     |        |        |        |      |       |   |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|---|
| ATOM | 2124 | CA  | ASP A | 300 | 22.930 | 31.636 | 29.950 | 1.00 | 10.66 | A |
| ATOM | 2125 | CB  | ASP A | 300 | 21.849 | 31.816 | 31.023 | 1.00 | 8.23  | A |
| ATOM | 2126 | CG  | ASP A | 300 | 22.055 | 30.877 | 32.193 | 1.00 | 14.11 | A |
| ATOM | 2127 | OD1 | ASP A | 300 | 22.141 | 29.660 | 31.928 | 1.00 | 8.23  | A |
| ATOM | 2128 | OD2 | ASP A | 300 | 22.149 | 31.341 | 33.373 | 1.00 | 15.65 | A |
| ATOM | 2129 | C   | ASP A | 300 | 22.828 | 32.790 | 28.975 | 1.00 | 10.65 | A |
| ATOM | 2130 | O   | ASP A | 300 | 23.690 | 33.669 | 28.931 | 1.00 | 8.49  | A |
| ATOM | 2131 | N   | LEU A | 301 | 21.740 | 32.765 | 28.202 | 1.00 | 8.77  | A |
| ATOM | 2132 | CA  | LEU A | 301 | 21.407 | 33.819 | 27.246 | 1.00 | 10.49 | A |
| ATOM | 2133 | CB  | LEU A | 301 | 21.121 | 33.226 | 25.850 | 1.00 | 10.57 | A |
| ATOM | 2134 | CG  | LEU A | 301 | 22.189 | 32.371 | 25.157 | 1.00 | 17.61 | A |
| ATOM | 2135 | CD1 | LEU A | 301 | 21.699 | 31.951 | 23.775 | 1.00 | 16.46 | A |
| ATOM | 2136 | CD2 | LEU A | 301 | 23.456 | 33.151 | 25.057 | 1.00 | 12.96 | A |
| ATOM | 2137 | C   | LEU A | 301 | 20.128 | 34.533 | 27.689 | 1.00 | 7.85  | A |
| ATOM | 2138 | O   | LEU A | 301 | 19.179 | 33.889 | 28.127 | 1.00 | 7.63  | A |
| ATOM | 2139 | N   | ILE A | 302 | 20.101 | 35.855 | 27.564 | 1.00 | 8.91  | A |
| ATOM | 2140 | CA  | ILE A | 302 | 18.897 | 36.614 | 27.879 | 1.00 | 7.82  | A |
| ATOM | 2141 | CB  | ILE A | 302 | 19.146 | 37.648 | 29.000 | 1.00 | 10.36 | A |
| ATOM | 2142 | CG2 | ILE A | 302 | 17.848 | 38.429 | 29.261 | 1.00 | 12.51 | A |
| ATOM | 2143 | CG1 | ILE A | 302 | 19.588 | 36.918 | 30.287 | 1.00 | 8.81  | A |
| ATOM | 2144 | CD1 | ILE A | 302 | 20.089 | 37.867 | 31.411 | 1.00 | 7.82  | A |
| ATOM | 2145 | C   | ILE A | 302 | 18.517 | 37.368 | 26.602 | 1.00 | 9.48  | A |
| ATOM | 2146 | O   | ILE A | 302 | 19.320 | 38.158 | 26.096 | 1.00 | 8.44  | A |
| ATOM | 2147 | N   | PHE A | 303 | 17.311 | 37.120 | 26.081 | 1.00 | 8.80  | A |
| ATOM | 2148 | CA  | PHE A | 303 | 16.843 | 37.786 | 24.854 | 1.00 | 8.37  | A |
| ATOM | 2149 | CB  | PHE A | 303 | 16.751 | 36.821 | 23.651 | 1.00 | 7.07  | A |
| ATOM | 2150 | CG  | PHE A | 303 | 18.054 | 36.583 | 22.944 | 1.00 | 8.30  | A |
| ATOM | 2151 | CD1 | PHE A | 303 | 19.027 | 35.770 | 23.500 | 1.00 | 8.48  | A |
| ATOM | 2152 | CD2 | PHE A | 303 | 18.316 | 37.205 | 21.725 | 1.00 | 7.08  | A |
| ATOM | 2153 | CE1 | PHE A | 303 | 20.265 | 35.582 | 22.851 | 1.00 | 7.30  | A |
| ATOM | 2154 | CE2 | PHE A | 303 | 19.559 | 37.023 | 21.065 | 1.00 | 9.28  | A |
| ATOM | 2155 | CZ  | PHE A | 303 | 20.528 | 36.210 | 21.637 | 1.00 | 11.64 | A |
| ATOM | 2156 | C   | PHE A | 303 | 15.437 | 38.305 | 25.032 | 1.00 | 9.03  | A |
| ATOM | 2157 | O   | PHE A | 303 | 14.797 | 38.052 | 26.031 | 1.00 | 9.30  | A |
| ATOM | 2158 | N   | SER A | 304 | 14.947 | 39.002 | 24.014 | 1.00 | 7.56  | A |
| ATOM | 2159 | CA  | SER A | 304 | 13.566 | 39.465 | 24.044 | 1.00 | 9.72  | A |
| ATOM | 2160 | CB  | SER A | 304 | 13.470 | 40.870 | 23.444 | 1.00 | 11.08 | A |
| ATOM | 2161 | OG  | SER A | 304 | 12.117 | 41.291 | 23.498 | 1.00 | 10.08 | A |
| ATOM | 2162 | C   | SER A | 304 | 12.707 | 38.530 | 23.170 | 1.00 | 6.80  | A |
| ATOM | 2163 | O   | SER A | 304 | 13.198 | 38.018 | 22.162 | 1.00 | 10.90 | A |
| ATOM | 2164 | N   | GLU A | 305 | 11.451 | 38.293 | 23.534 | 1.00 | 8.14  | A |
| ATOM | 2165 | CA  | GLU A | 305 | 10.605 | 37.482 | 22.655 | 1.00 | 11.11 | A |
| ATOM | 2166 | CB  | GLU A | 305 | 9.268  | 37.125 | 23.316 | 1.00 | 10.66 | A |
| ATOM | 2167 | CG  | GLU A | 305 | 8.447  | 36.161 | 22.439 | 1.00 | 11.71 | A |
| ATOM | 2168 | CD  | GLU A | 305 | 7.073  | 35.820 | 22.985 | 1.00 | 12.77 | A |
| ATOM | 2169 | OE1 | GLU A | 305 | 6.767  | 36.154 | 24.147 | 1.00 | 14.12 | A |
| ATOM | 2170 | OE2 | GLU A | 305 | 6.288  | 35.192 | 22.228 | 1.00 | 16.70 | A |
| ATOM | 2171 | C   | GLU A | 305 | 10.305 | 38.329 | 21.399 | 1.00 | 15.34 | A |
| ATOM | 2172 | O   | GLU A | 305 | 10.154 | 37.800 | 20.283 | 1.00 | 10.74 | A |
| ATOM | 2173 | N   | CYS A | 306 | 10.239 | 39.649 | 21.574 | 1.00 | 11.86 | A |
| ATOM | 2174 | CA  | CYS A | 306 | 9.889  | 40.534 | 20.450 | 1.00 | 12.96 | A |
| ATOM | 2175 | C   | CYS A | 306 | 10.859 | 41.666 | 20.140 | 1.00 | 14.14 | A |
| ATOM | 2176 | O   | CYS A | 306 | 11.434 | 42.270 | 21.046 | 1.00 | 11.98 | A |
| ATOM | 2177 | CB  | CYS A | 306 | 8.531  | 41.185 | 20.726 | 1.00 | 11.40 | A |
| ATOM | 2178 | SG  | CYS A | 306 | 7.188  | 40.111 | 21.313 | 1.00 | 15.63 | A |
| ATOM | 2179 | N   | TYR A | 307 | 11.017 | 41.956 | 18.854 | 1.00 | 12.82 | A |
| ATOM | 2180 | CA  | TYR A | 307 | 11.872 | 43.060 | 18.397 | 1.00 | 10.85 | A |
| ATOM | 2181 | CB  | TYR A | 307 | 13.143 | 42.533 | 17.712 | 1.00 | 8.88  | A |
| ATOM | 2182 | CG  | TYR A | 307 | 14.066 | 41.850 | 18.703 | 1.00 | 13.96 | A |
| ATOM | 2183 | CD1 | TYR A | 307 | 13.902 | 40.499 | 19.020 | 1.00 | 13.44 | A |
| ATOM | 2184 | CE1 | TYR A | 307 | 14.683 | 39.882 | 20.020 | 1.00 | 13.43 | A |
| ATOM | 2185 | CD2 | TYR A | 307 | 15.035 | 42.579 | 19.401 | 1.00 | 11.32 | A |
| ATOM | 2186 | CE2 | TYR A | 307 | 15.821 | 41.972 | 20.410 | 1.00 | 11.99 | A |
| ATOM | 2187 | CZ  | TYR A | 307 | 15.637 | 40.625 | 20.712 | 1.00 | 12.10 | A |
| ATOM | 2188 | OH  | TYR A | 307 | 16.379 | 40.019 | 21.724 | 1.00 | 12.32 | A |
| ATOM | 2189 | C   | TYR A | 307 | 11.056 | 43.908 | 17.424 | 1.00 | 13.04 | A |
| ATOM | 2190 | O   | TYR A | 307 | 10.318 | 43.370 | 16.588 | 1.00 | 11.71 | A |
| ATOM | 2191 | N   | ALA A | 308 | 11.161 | 45.229 | 17.546 | 1.00 | 13.47 | A |
| ATOM | 2192 | CA  | ALA A | 308 | 10.420 | 46.123 | 16.660 | 1.00 | 19.16 | A |
| ATOM | 2193 | CB  | ALA A | 308 | 10.623 | 47.583 | 17.116 | 1.00 | 19.39 | A |
| ATOM | 2194 | C   | ALA A | 308 | 10.827 | 45.960 | 15.176 | 1.00 | 16.58 | A |
| ATOM | 2195 | O   | ALA A | 308 | 9.990  | 46.011 | 14.290 | 1.00 | 15.94 | A |
| ATOM | 2196 | N   | ASN A | 309 | 12.109 | 45.752 | 14.919 | 1.00 | 16.56 | A |
| ATOM | 2197 | CA  | ASN A | 309 | 12.621 | 45.602 | 13.565 | 1.00 | 15.71 | A |
| ATOM | 2198 | CB  | ASN A | 309 | 14.084 | 46.052 | 13.558 | 1.00 | 11.74 | A |
| ATOM | 2199 | CG  | ASN A | 309 | 14.704 | 46.002 | 12.183 | 1.00 | 20.62 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2200 | OD1 | ASN | A | 309 | 15.130 | 44.946 | 11.713 | 1.00 | 17.26 | A |
| ATOM | 2201 | ND2 | ASN | A | 309 | 14.741 | 47.153 | 11.517 | 1.00 | 13.84 | A |
| ATOM | 2202 | C   | ASN | A | 309 | 12.493 | 44.142 | 13.066 | 1.00 | 16.39 | A |
| ATOM | 2203 | O   | ASN | A | 309 | 13.031 | 43.221 | 13.678 | 1.00 | 11.54 | A |
| ATOM | 2204 | N   | ALA | A | 310 | 11.806 | 43.942 | 11.941 | 1.00 | 12.69 | A |
| ATOM | 2205 | CA  | ALA | A | 310 | 11.583 | 42.584 | 11.430 | 1.00 | 16.06 | A |
| ATOM | 2206 | CB  | ALA | A | 310 | 10.564 | 42.618 | 10.281 | 1.00 | 16.44 | A |
| ATOM | 2207 | C   | ALA | A | 310 | 12.836 | 41.828 | 10.997 | 1.00 | 14.76 | A |
| ATOM | 2208 | O   | ALA | A | 310 | 12.907 | 40.599 | 11.128 | 1.00 | 15.90 | A |
| ATOM | 2209 | N   | THR | A | 311 | 13.827 | 42.546 | 10.485 | 1.00 | 13.61 | A |
| ATOM | 2210 | CA  | THR | A | 311 | 15.074 | 41.922 | 10.069 | 1.00 | 14.28 | A |
| ATOM | 2211 | CB  | THR | A | 311 | 15.949 | 42.927 | 9.314  | 1.00 | 15.47 | A |
| ATOM | 2212 | OG1 | THR | A | 311 | 15.284 | 43.307 | 8.097  | 1.00 | 18.10 | A |
| ATOM | 2213 | CG2 | THR | A | 311 | 17.291 | 42.322 | 8.977  | 1.00 | 16.40 | A |
| ATOM | 2214 | C   | THR | A | 311 | 15.813 | 41.407 | 11.324 | 1.00 | 15.00 | A |
| ATOM | 2215 | O   | THR | A | 311 | 16.371 | 40.313 | 11.318 | 1.00 | 12.29 | A |
| ATOM | 2216 | N   | GLN | A | 312 | 15.798 | 42.180 | 12.409 | 1.00 | 13.08 | A |
| ATOM | 2217 | CA  | GLN | A | 312 | 16.477 | 41.717 | 13.623 | 1.00 | 12.35 | A |
| ATOM | 2218 | CB  | GLN | A | 312 | 16.545 | 42.827 | 14.682 | 1.00 | 10.08 | A |
| ATOM | 2219 | CG  | GLN | A | 312 | 17.501 | 43.960 | 14.273 | 1.00 | 7.89  | A |
| ATOM | 2220 | CD  | GLN | A | 312 | 17.696 | 44.997 | 15.377 | 1.00 | 13.93 | A |
| ATOM | 2221 | OE1 | GLN | A | 312 | 16.897 | 45.087 | 16.311 | 1.00 | 14.28 | A |
| ATOM | 2222 | NE2 | GLN | A | 312 | 18.743 | 45.799 | 15.255 | 1.00 | 16.18 | A |
| ATOM | 2223 | C   | GLN | A | 312 | 15.768 | 40.486 | 14.191 | 1.00 | 11.19 | A |
| ATOM | 2224 | O   | GLN | A | 312 | 16.418 | 39.537 | 14.639 | 1.00 | 14.09 | A |
| ATOM | 2225 | N   | THR | A | 313 | 14.439 | 40.507 | 14.189 | 1.00 | 9.72  | A |
| ATOM | 2226 | CA  | THR | A | 313 | 13.670 | 39.363 | 14.685 | 1.00 | 8.88  | A |
| ATOM | 2227 | CB  | THR | A | 313 | 12.149 | 39.541 | 14.449 | 1.00 | 13.95 | A |
| ATOM | 2228 | OG1 | THR | A | 313 | 11.660 | 40.660 | 15.197 | 1.00 | 14.46 | A |
| ATOM | 2229 | CG2 | THR | A | 313 | 11.398 | 38.288 | 14.832 | 1.00 | 12.76 | A |
| ATOM | 2230 | C   | THR | A | 313 | 14.108 | 38.096 | 13.935 | 1.00 | 10.80 | A |
| ATOM | 2231 | O   | THR | A | 313 | 14.318 | 37.042 | 14.538 | 1.00 | 11.41 | A |
| ATOM | 2232 | N   | GLY | A | 314 | 14.218 | 38.204 | 12.615 | 1.00 | 11.55 | A |
| ATOM | 2233 | CA  | GLY | A | 314 | 14.628 | 37.067 | 11.810 | 1.00 | 12.96 | A |
| ATOM | 2234 | C   | GLY | A | 314 | 16.060 | 36.638 | 12.090 | 1.00 | 10.31 | A |
| ATOM | 2235 | O   | GLY | A | 314 | 16.370 | 35.439 | 12.111 | 1.00 | 11.80 | A |
| ATOM | 2236 | N   | GLN | A | 315 | 16.952 | 37.603 | 12.291 | 1.00 | 10.00 | A |
| ATOM | 2237 | CA  | GLN | A | 315 | 18.360 | 37.280 | 12.586 | 1.00 | 10.98 | A |
| ATOM | 2238 | CB  | GLN | A | 315 | 19.219 | 38.542 | 12.512 | 1.00 | 12.34 | A |
| ATOM | 2239 | CG  | GLN | A | 315 | 19.286 | 39.069 | 11.071 | 1.00 | 13.86 | A |
| ATOM | 2240 | CD  | GLN | A | 315 | 20.014 | 40.385 | 10.558 | 1.00 | 16.05 | A |
| ATOM | 2241 | OE1 | GLN | A | 315 | 19.868 | 41.254 | 11.818 | 1.00 | 15.65 | A |
| ATOM | 2242 | NE2 | GLN | A | 315 | 20.787 | 40.552 | 9.880  | 1.00 | 15.34 | A |
| ATOM | 2243 | C   | GLN | A | 315 | 18.518 | 36.613 | 13.952 | 1.00 | 11.33 | A |
| ATOM | 2244 | O   | GLN | A | 315 | 19.385 | 35.743 | 14.136 | 1.00 | 12.86 | A |
| ATOM | 2245 | N   | VAL | A | 316 | 17.677 | 37.006 | 14.909 | 1.00 | 11.99 | A |
| ATOM | 2246 | CA  | VAL | A | 316 | 17.719 | 36.389 | 16.238 | 1.00 | 11.29 | A |
| ATOM | 2247 | CB  | VAL | A | 316 | 16.803 | 37.131 | 17.251 | 1.00 | 12.97 | A |
| ATOM | 2248 | CG1 | VAL | A | 316 | 16.658 | 36.292 | 18.541 | 1.00 | 12.95 | A |
| ATOM | 2249 | CG2 | VAL | A | 316 | 17.401 | 38.493 | 17.502 | 1.00 | 11.75 | A |
| ATOM | 2250 | C   | VAL | A | 316 | 17.232 | 34.929 | 16.092 | 1.00 | 13.11 | A |
| ATOM | 2251 | O   | VAL | A | 316 | 17.813 | 33.996 | 16.667 | 1.00 | 12.64 | A |
| ATOM | 2252 | N   | ARG | A | 317 | 16.154 | 34.723 | 15.327 | 1.00 | 9.04  | A |
| ATOM | 2253 | CA  | ARG | A | 317 | 15.672 | 33.364 | 15.115 | 1.00 | 12.87 | A |
| ATOM | 2254 | CB  | ARG | A | 317 | 14.348 | 33.372 | 14.303 | 1.00 | 14.06 | A |
| ATOM | 2255 | CG  | ARG | A | 317 | 13.148 | 33.951 | 15.076 | 1.00 | 13.07 | A |
| ATOM | 2256 | CD  | ARG | A | 317 | 11.823 | 33.964 | 14.243 | 1.00 | 14.93 | A |
| ATOM | 2257 | NE  | ARG | A | 317 | 11.520 | 32.611 | 13.755 | 1.00 | 14.57 | A |
| ATOM | 2258 | CZ  | ARG | A | 317 | 10.894 | 31.677 | 14.480 | 1.00 | 10.03 | A |
| ATOM | 2259 | NH1 | ARG | A | 317 | 10.470 | 31.934 | 15.704 | 1.00 | 9.62  | A |
| ATOM | 2260 | NH2 | ARG | A | 317 | 10.730 | 30.461 | 13.983 | 1.00 | 13.56 | A |
| ATOM | 2261 | C   | ARG | A | 317 | 16.730 | 32.491 | 14.434 | 1.00 | 12.01 | A |
| ATOM | 2262 | O   | ARG | A | 317 | 16.879 | 31.320 | 14.783 | 1.00 | 12.09 | A |
| ATOM | 2263 | N   | ASN | A | 318 | 17.462 | 33.033 | 13.464 | 1.00 | 11.68 | A |
| ATOM | 2264 | CA  | ASN | A | 318 | 18.503 | 32.246 | 12.796 | 1.00 | 13.18 | A |
| ATOM | 2265 | CB  | ASN | A | 318 | 19.123 | 33.028 | 11.629 | 1.00 | 11.52 | A |
| ATOM | 2266 | CG  | ASN | A | 318 | 18.145 | 33.249 | 10.500 | 1.00 | 15.15 | A |
| ATOM | 2267 | OD1 | ASN | A | 318 | 17.140 | 32.557 | 10.402 | 1.00 | 13.70 | A |
| ATOM | 2268 | ND2 | ASN | A | 318 | 18.438 | 34.211 | 9.638  | 1.00 | 17.31 | A |
| ATOM | 2269 | C   | ASN | A | 318 | 19.613 | 31.841 | 13.771 | 1.00 | 12.19 | A |
| ATOM | 2270 | O   | ASN | A | 318 | 20.207 | 30.753 | 13.658 | 1.00 | 9.01  | A |
| ATOM | 2271 | N   | PHE | A | 319 | 19.904 | 32.715 | 14.733 | 1.00 | 10.68 | A |
| ATOM | 2272 | CA  | PHE | A | 319 | 20.936 | 32.376 | 15.707 | 1.00 | 9.90  | A |
| ATOM | 2273 | CB  | PHE | A | 319 | 21.274 | 33.577 | 16.584 | 1.00 | 7.66  | A |
| ATOM | 2274 | CG  | PHE | A | 319 | 22.105 | 33.212 | 17.794 | 1.00 | 10.09 | A |
| ATOM | 2275 | CD1 | PHE | A | 319 | 23.351 | 32.644 | 17.631 | 1.00 | 6.01  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2276 | CD2 | PHE | A | 319 | 21.593 | 33.356 | 19.087 | 1.00 | 10.54 | A |
| ATOM | 2277 | CE1 | PHE | A | 319 | 24.102 | 32.203 | 18.738 | 1.00 | 12.72 | A |
| ATOM | 2278 | CE2 | PHE | A | 319 | 22.333 | 32.919 | 20.212 | 1.00 | 15.07 | A |
| ATOM | 2279 | CZ  | PHE | A | 319 | 23.589 | 32.338 | 20.027 | 1.00 | 12.59 | A |
| ATOM | 2280 | C   | PHE | A | 319 | 20.449 | 31.222 | 16.587 | 1.00 | 10.27 | A |
| ATOM | 2281 | O   | PHE | A | 319 | 21.203 | 30.282 | 16.868 | 1.00 | 12.47 | A |
| ATOM | 2282 | N   | PHE | A | 320 | 19.188 | 31.275 | 17.013 | 1.00 | 10.21 | A |
| ATOM | 2283 | CA  | PHE | A | 320 | 18.649 | 30.213 | 17.860 | 1.00 | 10.79 | A |
| ATOM | 2284 | CB  | PHE | A | 320 | 17.247 | 30.581 | 18.363 | 1.00 | 9.11  | A |
| ATOM | 2285 | CG  | PHE | A | 320 | 17.246 | 31.285 | 19.698 | 1.00 | 7.96  | A |
| ATOM | 2286 | CD1 | PHE | A | 320 | 16.762 | 30.642 | 20.833 | 1.00 | 9.52  | A |
| ATOM | 2287 | CD2 | PHE | A | 320 | 17.723 | 32.583 | 19.822 | 1.00 | 12.60 | A |
| ATOM | 2288 | CE1 | PHE | A | 320 | 16.750 | 31.282 | 22.082 | 1.00 | 6.69  | A |
| ATOM | 2289 | CE2 | PHE | A | 320 | 17.712 | 33.244 | 21.075 | 1.00 | 9.45  | A |
| ATOM | 2290 | CZ  | PHE | A | 320 | 17.220 | 32.579 | 22.209 | 1.00 | 8.89  | A |
| ATOM | 2291 | C   | PHE | A | 320 | 18.598 | 28.912 | 17.089 | 1.00 | 7.76  | A |
| ATOM | 2292 | O   | PHE | A | 320 | 18.856 | 27.838 | 17.634 | 1.00 | 9.90  | A |
| ATOM | 2293 | N   | THR | A | 321 | 18.274 | 29.013 | 15.801 | 1.00 | 8.04  | A |
| ATOM | 2294 | CA  | THR | A | 321 | 18.199 | 27.829 | 14.950 | 1.00 | 6.79  | A |
| ATOM | 2295 | CB  | THR | A | 321 | 17.687 | 28.224 | 13.551 | 1.00 | 7.01  | A |
| ATOM | 2296 | OG1 | THR | A | 321 | 16.334 | 28.695 | 13.691 | 1.00 | 11.25 | A |
| ATOM | 2297 | CG2 | THR | A | 321 | 17.731 | 27.032 | 12.573 | 1.00 | 9.32  | A |
| ATOM | 2298 | C   | THR | A | 321 | 19.535 | 27.128 | 14.872 | 1.00 | 11.09 | A |
| ATOM | 2299 | O   | THR | A | 321 | 19.594 | 25.896 | 14.823 | 1.00 | 10.46 | A |
| ATOM | 2300 | N   | LYS | A | 322 | 20.617 | 27.904 | 14.873 | 1.00 | 8.41  | A |
| ATOM | 2301 | CA  | LYS | A | 322 | 21.950 | 27.319 | 14.849 | 1.00 | 8.00  | A |
| ATOM | 2302 | CB  | LYS | A | 322 | 22.970 | 28.329 | 14.299 | 1.00 | 6.38  | A |
| ATOM | 2303 | CG  | LYS | A | 322 | 24.410 | 27.805 | 14.359 | 1.00 | 10.15 | A |
| ATOM | 2304 | CD  | LYS | A | 322 | 25.396 | 28.712 | 13.615 | 1.00 | 8.08  | A |
| ATOM | 2305 | CE  | LYS | A | 322 | 26.665 | 27.922 | 13.317 | 1.00 | 11.78 | A |
| ATOM | 2306 | NZ  | LYS | A | 322 | 27.577 | 28.702 | 12.437 | 1.00 | 18.79 | A |
| ATOM | 2307 | C   | LYS | A | 322 | 22.415 | 26.857 | 16.242 | 1.00 | 9.52  | A |
| ATOM | 2308 | O   | LYS | A | 322 | 22.864 | 25.711 | 16.425 | 1.00 | 9.02  | A |
| ATOM | 2309 | N   | HIS | A | 323 | 22.289 | 27.735 | 17.231 | 1.00 | 10.06 | A |
| ATOM | 2310 | CA  | HIS | A | 323 | 22.793 | 27.420 | 18.569 | 1.00 | 9.00  | A |
| ATOM | 2311 | CB  | HIS | A | 323 | 22.710 | 28.677 | 19.469 | 1.00 | 7.78  | A |
| ATOM | 2312 | CG  | HIS | A | 323 | 23.655 | 28.657 | 20.637 | 1.00 | 9.56  | A |
| ATOM | 2313 | CD2 | HIS | A | 323 | 23.426 | 28.762 | 21.970 | 1.00 | 9.53  | A |
| ATOM | 2314 | ND1 | HIS | A | 323 | 25.028 | 28.560 | 20.494 | 1.00 | 7.88  | A |
| ATOM | 2315 | CE1 | HIS | A | 323 | 25.602 | 28.615 | 21.683 | 1.00 | 9.47  | A |
| ATOM | 2316 | NE2 | HIS | A | 323 | 24.653 | 28.736 | 22.598 | 1.00 | 12.97 | A |
| ATOM | 2317 | C   | HIS | A | 323 | 22.082 | 26.230 | 19.222 | 1.00 | 9.52  | A |
| ATOM | 2318 | O   | HIS | A | 323 | 22.687 | 25.507 | 20.019 | 1.00 | 8.65  | A |
| ATOM | 2319 | N   | TYR | A | 324 | 20.808 | 26.034 | 18.877 | 1.00 | 9.61  | A |
| ATOM | 2320 | CA  | TYR | A | 324 | 20.024 | 24.911 | 19.427 | 1.00 | 10.38 | A |
| ATOM | 2321 | CB  | TYR | A | 324 | 18.767 | 25.434 | 20.149 | 1.00 | 6.95  | A |
| ATOM | 2322 | CG  | TYR | A | 324 | 19.137 | 26.376 | 21.277 | 1.00 | 7.33  | A |
| ATOM | 2323 | CD1 | TYR | A | 324 | 19.195 | 27.752 | 21.072 | 1.00 | 5.99  | A |
| ATOM | 2324 | CE1 | TYR | A | 324 | 19.656 | 28.618 | 22.097 | 1.00 | 8.99  | A |
| ATOM | 2325 | CD2 | TYR | A | 324 | 19.533 | 25.882 | 22.513 | 1.00 | 7.61  | A |
| ATOM | 2326 | CE2 | TYR | A | 324 | 19.994 | 26.731 | 23.525 | 1.00 | 5.98  | A |
| ATOM | 2327 | CZ  | TYR | A | 324 | 20.052 | 28.094 | 23.303 | 1.00 | 7.54  | A |
| ATOM | 2328 | OH  | TYR | A | 324 | 20.547 | 28.926 | 24.294 | 1.00 | 7.56  | A |
| ATOM | 2329 | C   | TYR | A | 324 | 19.627 | 23.893 | 18.338 | 1.00 | 7.02  | A |
| ATOM | 2330 | O   | TYR | A | 324 | 18.677 | 23.118 | 18.498 | 1.00 | 10.94 | A |
| ATOM | 2331 | N   | GLY | A | 325 | 20.387 | 23.868 | 17.254 | 1.00 | 7.94  | A |
| ATOM | 2332 | CA  | GLY | A | 325 | 20.064 | 22.938 | 16.181 | 1.00 | 7.51  | A |
| ATOM | 2333 | C   | GLY | A | 325 | 20.514 | 21.493 | 16.386 | 1.00 | 12.01 | A |
| ATOM | 2334 | O   | GLY | A | 325 | 21.492 | 21.227 | 17.097 | 1.00 | 10.59 | A |
| ATOM | 2335 | N   | THR | A | 326 | 19.788 | 20.564 | 15.752 | 1.00 | 8.75  | A |
| ATOM | 2336 | CA  | THR | A | 326 | 20.113 | 19.132 | 15.790 | 1.00 | 10.25 | A |
| ATOM | 2337 | CB  | THR | A | 326 | 19.005 | 18.311 | 15.135 | 1.00 | 9.46  | A |
| ATOM | 2338 | OG1 | THR | A | 326 | 17.759 | 18.707 | 15.708 | 1.00 | 10.73 | A |
| ATOM | 2339 | CG2 | THR | A | 326 | 19.212 | 16.788 | 15.369 | 1.00 | 7.67  | A |
| ATOM | 2340 | C   | THR | A | 326 | 21.432 | 18.937 | 15.038 | 1.00 | 9.78  | A |
| ATOM | 2341 | O   | THR | A | 326 | 22.278 | 18.131 | 15.452 | 1.00 | 10.90 | A |
| ATOM | 2342 | N   | SER | A | 327 | 21.614 | 19.688 | 13.953 | 1.00 | 12.37 | A |
| ATOM | 2343 | CA  | SER | A | 327 | 22.858 | 19.666 | 13.176 | 1.00 | 11.58 | A |
| ATOM | 2344 | CB  | SER | A | 327 | 22.743 | 18.752 | 11.935 | 1.00 | 14.65 | A |
| ATOM | 2345 | OG  | SER | A | 327 | 21.725 | 19.192 | 11.051 | 1.00 | 10.13 | A |
| ATOM | 2346 | C   | SER | A | 327 | 23.158 | 21.118 | 12.764 | 1.00 | 10.87 | A |
| ATOM | 2347 | O   | SER | A | 327 | 22.419 | 22.031 | 13.149 | 1.00 | 9.05  | A |
| ATOM | 2348 | N   | ALA | A | 328 | 24.228 | 21.331 | 12.000 | 1.00 | 11.22 | A |
| ATOM | 2349 | CA  | ALA | A | 328 | 24.637 | 22.690 | 11.567 | 1.00 | 10.30 | A |
| ATOM | 2350 | CB  | ALA | A | 328 | 23.682 | 23.234 | 10.518 | 1.00 | 12.01 | A |
| ATOM | 2351 | C   | ALA | A | 328 | 24.602 | 23.592 | 12.790 | 1.00 | 11.88 | A |

FIGURE 5 (suite)

|      |      |     |       |     |        |        |        |      |       |   |
|------|------|-----|-------|-----|--------|--------|--------|------|-------|---|
| ATOM | 2352 | O   | ALA A | 328 | 24.046 | 24.674 | 12.742 | 1.00 | 13.69 | A |
| ATOM | 2353 | N   | ASN A | 329 | 25.197 | 23.140 | 13.887 | 1.00 | 11.26 | A |
| ATOM | 2354 | CA  | ASN A | 329 | 25.150 | 23.910 | 15.123 | 1.00 | 10.51 | A |
| ATOM | 2355 | CB  | ASN A | 329 | 24.422 | 23.083 | 16.205 | 1.00 | 8.81  | A |
| ATOM | 2356 | CG  | ASN A | 329 | 25.132 | 21.771 | 16.536 | 1.00 | 9.32  | A |
| ATOM | 2357 | OD1 | ASN A | 329 | 26.352 | 21.717 | 16.573 | 1.00 | 11.49 | A |
| ATOM | 2358 | ND2 | ASN A | 329 | 24.360 | 20.714 | 16.792 | 1.00 | 10.75 | A |
| ATOM | 2359 | C   | ASN A | 329 | 26.526 | 24.402 | 15.604 | 1.00 | 12.21 | A |
| ATOM | 2360 | O   | ASN A | 329 | 27.515 | 24.381 | 14.849 | 1.00 | 9.35  | A |
| ATOM | 2361 | N   | ASP A | 330 | 26.586 | 24.863 | 16.851 | 1.00 | 10.38 | A |
| ATOM | 2362 | CA  | ASP A | 330 | 27.837 | 25.386 | 17.412 | 1.00 | 9.41  | A |
| ATOM | 2363 | CB  | ASP A | 330 | 27.575 | 26.677 | 18.208 | 1.00 | 10.91 | A |
| ATOM | 2364 | CG  | ASP A | 330 | 27.239 | 27.852 | 17.331 | 1.00 | 13.71 | A |
| ATOM | 2365 | OD1 | ASP A | 330 | 26.333 | 28.653 | 17.720 | 1.00 | 14.93 | A |
| ATOM | 2366 | OD2 | ASP A | 330 | 27.880 | 27.981 | 16.261 | 1.00 | 10.16 | A |
| ATOM | 2367 | C   | ASP A | 330 | 28.536 | 24.416 | 18.346 | 1.00 | 10.31 | A |
| ATOM | 2368 | O   | ASP A | 330 | 29.484 | 24.809 | 19.029 | 1.00 | 8.29  | A |
| ATOM | 2369 | N   | ASN A | 331 | 28.111 | 23.153 | 18.363 | 1.00 | 8.79  | A |
| ATOM | 2370 | CA  | ASN A | 331 | 28.698 | 22.217 | 19.311 | 1.00 | 10.91 | A |
| ATOM | 2371 | CB  | ASN A | 331 | 27.942 | 20.869 | 19.267 | 1.00 | 11.40 | A |
| ATOM | 2372 | CG  | ASN A | 331 | 26.579 | 20.924 | 19.989 | 1.00 | 15.36 | A |
| ATOM | 2373 | OD1 | ASN A | 331 | 25.926 | 19.893 | 20.194 | 1.00 | 12.09 | A |
| ATOM | 2374 | ND2 | ASN A | 331 | 26.156 | 22.115 | 20.372 | 1.00 | 9.71  | A |
| ATOM | 2375 | C   | ASN A | 331 | 30.220 | 22.012 | 19.218 | 1.00 | 12.28 | A |
| ATOM | 2376 | O   | ASN A | 331 | 30.877 | 21.866 | 20.255 | 1.00 | 12.57 | A |
| ATOM | 2377 | N   | ALA A | 332 | 30.795 | 22.001 | 18.012 | 1.00 | 10.00 | A |
| ATOM | 2378 | CA  | ALA A | 332 | 32.252 | 21.842 | 17.903 | 1.00 | 12.41 | A |
| ATOM | 2379 | CB  | ALA A | 332 | 32.677 | 21.733 | 16.445 | 1.00 | 12.06 | A |
| ATOM | 2380 | C   | ALA A | 332 | 32.964 | 23.028 | 18.548 | 1.00 | 8.53  | A |
| ATOM | 2381 | O   | ALA A | 332 | 33.973 | 22.872 | 19.247 | 1.00 | 11.75 | A |
| ATOM | 2382 | N   | ALA A | 333 | 32.447 | 24.216 | 18.297 | 1.00 | 9.64  | A |
| ATOM | 2383 | CA  | ALA A | 333 | 33.057 | 25.422 | 18.858 | 1.00 | 10.83 | A |
| ATOM | 2384 | CB  | ALA A | 333 | 32.424 | 26.655 | 18.223 | 1.00 | 9.42  | A |
| ATOM | 2385 | C   | ALA A | 333 | 32.910 | 25.473 | 20.379 | 1.00 | 10.44 | A |
| ATOM | 2386 | O   | ALA A | 333 | 33.787 | 25.982 | 21.096 | 1.00 | 9.81  | A |
| ATOM | 2387 | N   | ILE A | 334 | 31.787 | 24.963 | 20.869 | 1.00 | 9.49  | A |
| ATOM | 2388 | CA  | ILE A | 334 | 31.536 | 24.919 | 22.305 | 1.00 | 10.34 | A |
| ATOM | 2389 | CB  | ILE A | 334 | 30.099 | 24.404 | 22.567 | 1.00 | 7.35  | A |
| ATOM | 2390 | CG2 | ILE A | 334 | 29.902 | 24.030 | 24.056 | 1.00 | 4.48  | A |
| ATOM | 2391 | CG1 | ILE A | 334 | 29.093 | 25.467 | 22.091 | 1.00 | 8.68  | A |
| ATOM | 2392 | CD1 | ILE A | 334 | 27.628 | 24.953 | 22.043 | 1.00 | 8.29  | A |
| ATOM | 2393 | C   | ILE A | 334 | 32.593 | 24.003 | 22.946 | 1.00 | 9.03  | A |
| ATOM | 2394 | O   | ILE A | 334 | 33.239 | 24.352 | 23.954 | 1.00 | 6.82  | A |
| ATOM | 2395 | N   | GLN A | 335 | 32.805 | 22.847 | 22.333 | 1.00 | 6.99  | A |
| ATOM | 2396 | CA  | GLN A | 335 | 33.800 | 21.903 | 22.831 | 1.00 | 8.99  | A |
| ATOM | 2397 | CB  | GLN A | 335 | 33.695 | 20.589 | 22.053 | 1.00 | 11.58 | A |
| ATOM | 2398 | CG  | GLN A | 335 | 32.448 | 19.784 | 22.446 | 1.00 | 21.44 | A |
| ATOM | 2399 | CD  | GLN A | 335 | 32.279 | 18.518 | 21.598 | 1.00 | 30.71 | A |
| ATOM | 2400 | OE1 | GLN A | 335 | 33.212 | 18.083 | 20.927 | 1.00 | 34.68 | A |
| ATOM | 2401 | NE2 | GLN A | 335 | 31.089 | 17.926 | 21.638 | 1.00 | 37.34 | A |
| ATOM | 2402 | C   | GLN A | 335 | 35.223 | 22.438 | 22.774 | 1.00 | 12.27 | A |
| ATOM | 2403 | O   | GLN A | 335 | 36.014 | 22.219 | 23.704 | 1.00 | 10.25 | A |
| ATOM | 2404 | N   | ALA A | 336 | 35.547 | 23.143 | 21.690 | 1.00 | 10.75 | A |
| ATOM | 2405 | CA  | ALA A | 336 | 36.868 | 23.726 | 21.514 | 1.00 | 12.71 | A |
| ATOM | 2406 | CB  | ALA A | 336 | 36.989 | 24.375 | 20.091 | 1.00 | 9.35  | A |
| ATOM | 2407 | C   | ALA A | 336 | 37.109 | 24.794 | 22.591 | 1.00 | 11.11 | A |
| ATOM | 2408 | O   | ALA A | 336 | 38.247 | 25.134 | 22.894 | 1.00 | 11.00 | A |
| ATOM | 2409 | N   | ASN A | 337 | 36.025 | 25.310 | 23.164 | 1.00 | 8.06  | A |
| ATOM | 2410 | CA  | ASN A | 337 | 36.125 | 26.342 | 24.185 | 1.00 | 9.10  | A |
| ATOM | 2411 | CB  | ASN A | 337 | 35.098 | 27.440 | 23.887 | 1.00 | 8.86  | A |
| ATOM | 2412 | CG  | ASN A | 337 | 35.621 | 28.457 | 22.874 | 1.00 | 12.21 | A |
| ATOM | 2413 | OD1 | ASN A | 337 | 36.333 | 29.417 | 23.230 | 1.00 | 12.38 | A |
| ATOM | 2414 | ND2 | ASN A | 337 | 35.301 | 28.237 | 21.605 | 1.00 | 13.95 | A |
| ATOM | 2415 | C   | ASN A | 337 | 35.979 | 25.816 | 25.622 | 1.00 | 9.52  | A |
| ATOM | 2416 | O   | ASN A | 337 | 35.647 | 26.565 | 26.534 | 1.00 | 7.92  | A |
| ATOM | 2417 | N   | ALA A | 338 | 36.242 | 24.523 | 25.806 | 1.00 | 8.29  | A |
| ATOM | 2418 | CA  | ALA A | 338 | 36.194 | 23.863 | 27.117 | 1.00 | 8.92  | A |
| ATOM | 2419 | CB  | ALA A | 338 | 37.188 | 24.526 | 28.069 | 1.00 | 10.50 | A |
| ATOM | 2420 | C   | ALA A | 338 | 34.825 | 23.786 | 27.785 | 1.00 | 8.55  | A |
| ATOM | 2421 | O   | ALA A | 338 | 34.732 | 23.671 | 29.000 | 1.00 | 10.41 | A |
| ATOM | 2422 | N   | PHE A | 339 | 33.765 | 23.844 | 27.002 | 1.00 | 7.84  | A |
| ATOM | 2423 | CA  | PHE A | 339 | 32.410 | 23.781 | 27.553 | 1.00 | 8.93  | A |
| ATOM | 2424 | CB  | PHE A | 339 | 31.624 | 25.034 | 27.120 | 1.00 | 7.76  | A |
| ATOM | 2425 | CG  | PHE A | 339 | 32.258 | 26.345 | 27.576 | 1.00 | 10.23 | A |
| ATOM | 2426 | CD1 | PHE A | 339 | 32.566 | 26.557 | 28.923 | 1.00 | 11.28 | A |
| ATOM | 2427 | CD2 | PHE A | 339 | 32.497 | 27.369 | 26.664 | 1.00 | 9.75  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2428 | CE1 | PHE | A | 339 | 33.108 | 27.795 | 29.360 | 1.00 | 11.58 | A |
| ATOM | 2429 | CE2 | PHE | A | 339 | 33.033 | 28.613 | 27.077 | 1.00 | 8.17  | A |
| ATOM | 2430 | CZ  | PHE | A | 339 | 33.339 | 28.820 | 28.437 | 1.00 | 8.56  | A |
| ATOM | 2431 | C   | PHE | A | 339 | 31.647 | 22.514 | 27.151 | 1.00 | 9.93  | A |
| ATOM | 2432 | O   | PHE | A | 339 | 32.084 | 21.742 | 26.279 | 1.00 | 9.23  | A |
| ATOM | 2433 | N   | VAL | A | 340 | 30.506 | 22.304 | 27.797 | 1.00 | 8.19  | A |
| ATOM | 2434 | CA  | VAL | A | 340 | 29.669 | 21.139 | 27.531 | 1.00 | 10.26 | A |
| ATOM | 2435 | CB  | VAL | A | 340 | 29.169 | 20.468 | 28.851 | 1.00 | 11.72 | A |
| ATOM | 2436 | CG1 | VAL | A | 340 | 28.219 | 19.269 | 28.538 | 1.00 | 8.46  | A |
| ATOM | 2437 | CG2 | VAL | A | 340 | 30.346 | 19.998 | 29.679 | 1.00 | 8.91  | A |
| ATOM | 2438 | C   | VAL | A | 340 | 28.439 | 21.577 | 26.742 | 1.00 | 6.33  | A |
| ATOM | 2439 | O   | VAL | A | 340 | 27.675 | 22.433 | 27.186 | 1.00 | 6.81  | A |
| ATOM | 2440 | N   | PRO | A | 341 | 28.255 | 21.021 | 25.547 | 1.00 | 6.85  | A |
| ATOM | 2441 | CD  | PRO | A | 341 | 29.193 | 20.162 | 24.797 | 1.00 | 10.26 | A |
| ATOM | 2442 | CA  | PRO | A | 341 | 27.082 | 21.373 | 24.736 | 1.00 | 9.67  | A |
| ATOM | 2443 | CB  | PRO | A | 341 | 27.275 | 20.537 | 23.468 | 1.00 | 11.39 | A |
| ATOM | 2444 | CG  | PRO | A | 341 | 28.752 | 20.386 | 23.363 | 1.00 | 14.97 | A |
| ATOM | 2445 | C   | PRO | A | 341 | 25.807 | 20.931 | 25.497 | 1.00 | 10.96 | A |
| ATOM | 2446 | O   | PRO | A | 341 | 25.851 | 20.024 | 26.342 | 1.00 | 10.96 | A |
| ATOM | 2447 | N   | LEU | A | 342 | 24.673 | 21.558 | 25.211 | 1.00 | 8.13  | A |
| ATOM | 2448 | CA  | LEU | A | 342 | 23.435 | 21.157 | 25.870 | 1.00 | 10.08 | A |
| ATOM | 2449 | CB  | LEU | A | 342 | 22.326 | 22.194 | 25.646 | 1.00 | 12.81 | A |
| ATOM | 2450 | CG  | LEU | A | 342 | 22.558 | 23.605 | 26.207 | 1.00 | 16.13 | A |
| ATOM | 2451 | CD1 | LEU | A | 342 | 21.280 | 24.428 | 26.007 | 1.00 | 10.84 | A |
| ATOM | 2452 | CD2 | LEU | A | 342 | 22.908 | 23.542 | 27.715 | 1.00 | 14.00 | A |
| ATOM | 2453 | C   | LEU | A | 342 | 22.981 | 19.821 | 25.288 | 1.00 | 11.91 | A |
| ATOM | 2454 | O   | LEU | A | 342 | 23.142 | 19.565 | 24.072 | 1.00 | 10.04 | A |
| ATOM | 2455 | N   | PRO | A | 343 | 22.437 | 18.937 | 26.147 | 1.00 | 10.12 | A |
| ATOM | 2456 | CD  | PRO | A | 343 | 22.407 | 19.074 | 27.618 | 1.00 | 8.23  | A |
| ATOM | 2457 | CA  | PRO | A | 343 | 21.947 | 17.622 | 25.721 | 1.00 | 11.60 | A |
| ATOM | 2458 | CB  | PRO | A | 343 | 21.407 | 17.006 | 27.021 | 1.00 | 11.29 | A |
| ATOM | 2459 | CG  | PRO | A | 343 | 22.287 | 17.643 | 28.083 | 1.00 | 12.10 | A |
| ATOM | 2460 | C   | PRO | A | 343 | 20.850 | 17.839 | 24.688 | 1.00 | 11.38 | A |
| ATOM | 2461 | O   | PRO | A | 343 | 20.229 | 18.896 | 24.648 | 1.00 | 10.75 | A |
| ATOM | 2462 | N   | SER | A | 344 | 20.590 | 16.836 | 23.861 | 1.00 | 9.55  | A |
| ATOM | 2463 | CA  | SER | A | 344 | 19.592 | 16.995 | 22.801 | 1.00 | 8.34  | A |
| ATOM | 2464 | CB  | SER | A | 344 | 19.547 | 15.741 | 21.940 | 1.00 | 15.39 | A |
| ATOM | 2465 | OG  | SER | A | 344 | 19.245 | 14.625 | 22.760 | 1.00 | 23.25 | A |
| ATOM | 2466 | C   | SER | A | 344 | 18.185 | 17.315 | 23.281 | 1.00 | 8.79  | A |
| ATOM | 2467 | O   | SER | A | 344 | 17.474 | 18.051 | 22.615 | 1.00 | 11.06 | A |
| ATOM | 2468 | N   | ASN | A | 345 | 17.751 | 16.744 | 24.410 | 1.00 | 11.97 | A |
| ATOM | 2469 | CA  | ASN | A | 345 | 16.403 | 17.061 | 24.874 | 1.00 | 13.51 | A |
| ATOM | 2470 | CB  | ASN | A | 345 | 15.962 | 16.128 | 26.015 | 1.00 | 11.25 | A |
| ATOM | 2471 | CG  | ASN | A | 345 | 16.896 | 16.145 | 27.206 | 1.00 | 19.63 | A |
| ATOM | 2472 | OD1 | ASN | A | 345 | 18.105 | 16.399 | 27.083 | 1.00 | 15.65 | A |
| ATOM | 2473 | ND2 | ASN | A | 345 | 16.343 | 15.822 | 28.379 | 1.00 | 15.03 | A |
| ATOM | 2474 | C   | ASN | A | 345 | 16.296 | 18.532 | 25.277 | 1.00 | 12.03 | A |
| ATOM | 2475 | O   | ASN | A | 345 | 15.236 | 19.131 | 25.167 | 1.00 | 11.72 | A |
| ATOM | 2476 | N   | TRP | A | 346 | 17.397 | 19.115 | 25.739 | 1.00 | 10.97 | A |
| ATOM | 2477 | CA  | TRP | A | 346 | 17.397 | 20.533 | 26.097 | 1.00 | 9.55  | A |
| ATOM | 2478 | CB  | TRP | A | 346 | 18.663 | 20.890 | 26.881 | 1.00 | 8.50  | A |
| ATOM | 2479 | CG  | TRP | A | 346 | 18.475 | 20.695 | 28.372 | 1.00 | 9.10  | A |
| ATOM | 2480 | CD2 | TRP | A | 346 | 17.927 | 21.660 | 29.285 | 1.00 | 10.08 | A |
| ATOM | 2481 | CE2 | TRP | A | 346 | 17.831 | 21.036 | 30.549 | 1.00 | 12.11 | A |
| ATOM | 2482 | CE3 | TRP | A | 346 | 17.502 | 22.994 | 29.149 | 1.00 | 9.60  | A |
| ATOM | 2483 | CD1 | TRP | A | 346 | 18.694 | 19.553 | 29.099 | 1.00 | 9.06  | A |
| ATOM | 2484 | NE1 | TRP | A | 346 | 18.304 | 19.752 | 30.411 | 1.00 | 9.93  | A |
| ATOM | 2485 | CZ2 | TRP | A | 346 | 17.323 | 21.705 | 31.682 | 1.00 | 9.30  | A |
| ATOM | 2486 | CZ3 | TRP | A | 346 | 17.004 | 23.662 | 30.261 | 1.00 | 10.14 | A |
| ATOM | 2487 | CH2 | TRP | A | 346 | 16.917 | 23.012 | 31.522 | 1.00 | 12.99 | A |
| ATOM | 2488 | C   | TRP | A | 346 | 17.298 | 21.390 | 24.824 | 1.00 | 10.69 | A |
| ATOM | 2489 | O   | TRP | A | 346 | 16.509 | 22.333 | 24.769 | 1.00 | 13.16 | A |
| ATOM | 2490 | N   | LYS | A | 347 | 18.087 | 21.074 | 23.804 | 1.00 | 9.34  | A |
| ATOM | 2491 | CA  | LYS | A | 347 | 17.984 | 21.852 | 22.557 | 1.00 | 8.27  | A |
| ATOM | 2492 | CB  | LYS | A | 347 | 18.902 | 21.287 | 21.466 | 1.00 | 12.86 | A |
| ATOM | 2493 | CG  | LYS | A | 347 | 20.416 | 21.357 | 21.748 | 1.00 | 11.51 | A |
| ATOM | 2494 | CD  | LYS | A | 347 | 21.221 | 21.071 | 20.440 | 1.00 | 14.73 | A |
| ATOM | 2495 | CE  | LYS | A | 347 | 22.733 | 21.317 | 20.590 | 1.00 | 14.12 | A |
| ATOM | 2496 | NZ  | LYS | A | 347 | 23.467 | 20.312 | 21.462 | 1.00 | 10.37 | A |
| ATOM | 2497 | C   | LYS | A | 347 | 16.549 | 21.789 | 22.030 | 1.00 | 10.83 | A |
| ATOM | 2498 | O   | LYS | A | 347 | 15.956 | 22.814 | 21.631 | 1.00 | 8.78  | A |
| ATOM | 2499 | N   | ALA | A | 348 | 15.987 | 20.583 | 21.997 | 1.00 | 9.70  | A |
| ATOM | 2500 | CA  | ALA | A | 348 | 14.627 | 20.418 | 21.472 | 1.00 | 9.41  | A |
| ATOM | 2501 | CB  | ALA | A | 348 | 14.238 | 18.928 | 21.448 | 1.00 | 12.04 | A |
| ATOM | 2502 | C   | ALA | A | 348 | 13.589 | 21.224 | 22.251 | 1.00 | 10.82 | A |
| ATOM | 2503 | O   | ALA | A | 348 | 12.678 | 21.830 | 21.657 | 1.00 | 9.58  | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2504 | N   | ALA | A | 349 | 13.735 | 21.261 | 23.569 | 1.00 | 9.39  | A |
| ATOM | 2505 | CA  | ALA | A | 349 | 12.791 | 22.018 | 24.392 | 1.00 | 8.51  | A |
| ATOM | 2506 | CB  | ALA | A | 349 | 13.045 | 21.750 | 25.891 | 1.00 | 8.51  | A |
| ATOM | 2507 | C   | ALA | A | 349 | 12.909 | 23.518 | 24.095 | 1.00 | 10.22 | A |
| ATOM | 2508 | O   | ALA | A | 349 | 11.888 | 24.224 | 24.012 | 1.00 | 8.91  | A |
| ATOM | 2509 | N   | VAL | A | 350 | 14.140 | 24.002 | 23.930 | 1.00 | 12.16 | A |
| ATOM | 2510 | CA  | VAL | A | 350 | 14.347 | 25.423 | 23.649 | 1.00 | 8.94  | A |
| ATOM | 2511 | CB  | VAL | A | 350 | 15.863 | 25.794 | 23.629 | 1.00 | 8.30  | A |
| ATOM | 2512 | CG1 | VAL | A | 350 | 16.075 | 27.221 | 23.071 | 1.00 | 8.00  | A |
| ATOM | 2513 | CG2 | VAL | A | 350 | 16.439 | 25.729 | 25.075 | 1.00 | 8.81  | A |
| ATOM | 2514 | C   | VAL | A | 350 | 13.709 | 25.763 | 22.305 | 1.00 | 10.89 | A |
| ATOM | 2515 | O   | VAL | A | 350 | 13.046 | 26.787 | 22.177 | 1.00 | 11.46 | A |
| ATOM | 2516 | N   | ARG | A | 351 | 13.890 | 24.895 | 21.313 | 1.00 | 10.91 | A |
| ATOM | 2517 | CA  | ARG | A | 351 | 13.289 | 25.144 | 20.002 | 1.00 | 11.54 | A |
| ATOM | 2518 | CB  | ARG | A | 351 | 13.765 | 24.106 | 18.988 | 1.00 | 10.07 | A |
| ATOM | 2519 | CG  | ARG | A | 351 | 15.237 | 24.167 | 18.647 | 1.00 | 10.05 | A |
| ATOM | 2520 | CD  | ARG | A | 351 | 15.527 | 23.433 | 17.312 | 1.00 | 14.16 | A |
| ATOM | 2521 | NE  | ARG | A | 351 | 14.971 | 22.067 | 17.282 | 1.00 | 17.52 | A |
| ATOM | 2522 | CZ  | ARG | A | 351 | 15.577 | 20.991 | 17.780 | 1.00 | 14.15 | A |
| ATOM | 2523 | NH1 | ARG | A | 351 | 14.993 | 19.802 | 17.708 | 1.00 | 14.19 | A |
| ATOM | 2524 | NH2 | ARG | A | 351 | 16.775 | 21.097 | 18.338 | 1.00 | 15.54 | A |
| ATOM | 2525 | C   | ARG | A | 351 | 11.750 | 25.097 | 20.069 | 1.00 | 13.24 | A |
| ATOM | 2526 | O   | ARG | A | 351 | 11.061 | 25.925 | 19.477 | 1.00 | 10.64 | A |
| ATOM | 2527 | N   | ALA | A | 352 | 11.221 | 24.112 | 20.786 | 1.00 | 10.94 | A |
| ATOM | 2528 | CA  | ALA | A | 352 | 9.772  | 23.942 | 20.890 | 1.00 | 13.45 | A |
| ATOM | 2529 | CB  | ALA | A | 352 | 9.447  | 22.656 | 21.636 | 1.00 | 14.54 | A |
| ATOM | 2530 | C   | ALA | A | 352 | 9.028  | 25.112 | 21.527 | 1.00 | 14.05 | A |
| ATOM | 2531 | O   | ALA | A | 352 | 7.875  | 25.385 | 21.193 | 1.00 | 9.92  | A |
| ATOM | 2532 | N   | SER | A | 353 | 9.669  | 25.802 | 22.454 | 1.00 | 9.51  | A |
| ATOM | 2533 | CA  | SER | A | 353 | 9.024  | 26.932 | 23.094 | 1.00 | 10.39 | A |
| ATOM | 2534 | CB  | SER | A | 353 | 9.503  | 27.088 | 24.548 | 1.00 | 11.56 | A |
| ATOM | 2535 | OG  | SER | A | 353 | 8.802  | 26.220 | 25.436 | 1.00 | 14.83 | A |
| ATOM | 2536 | C   | SER | A | 353 | 9.308  | 28.245 | 22.386 | 1.00 | 12.07 | A |
| ATOM | 2537 | O   | SER | A | 353 | 8.403  | 29.033 | 22.178 | 1.00 | 12.33 | A |
| ATOM | 2538 | N   | TYR | A | 354 | 10.568 | 28.459 | 22.015 | 1.00 | 10.56 | A |
| ATOM | 2539 | CA  | TYR | A | 354 | 10.955 | 29.733 | 21.455 | 1.00 | 8.65  | A |
| ATOM | 2540 | CB  | TYR | A | 354 | 12.240 | 30.188 | 22.159 | 1.00 | 11.42 | A |
| ATOM | 2541 | CG  | TYR | A | 354 | 12.077 | 30.164 | 23.670 | 1.00 | 11.26 | A |
| ATOM | 2542 | CD1 | TYR | A | 354 | 11.168 | 31.007 | 24.296 | 1.00 | 11.16 | A |
| ATOM | 2543 | CE1 | TYR | A | 354 | 10.962 | 30.955 | 25.673 | 1.00 | 13.86 | A |
| ATOM | 2544 | CD2 | TYR | A | 354 | 12.795 | 29.265 | 24.455 | 1.00 | 12.94 | A |
| ATOM | 2545 | CE2 | TYR | A | 354 | 12.608 | 29.204 | 25.846 | 1.00 | 13.83 | A |
| ATOM | 2546 | CZ  | TYR | A | 354 | 11.692 | 30.048 | 26.437 | 1.00 | 15.93 | A |
| ATOM | 2547 | OH  | TYR | A | 354 | 11.496 | 29.985 | 27.784 | 1.00 | 31.84 | A |
| ATOM | 2548 | C   | TYR | A | 354 | 11.069 | 29.882 | 19.951 | 1.00 | 11.12 | A |
| ATOM | 2549 | O   | TYR | A | 354 | 11.137 | 31.011 | 19.456 | 1.00 | 11.00 | A |
| ATOM | 2550 | N   | LEU | A | 355 | 11.097 | 28.778 | 19.218 | 1.00 | 9.87  | A |
| ATOM | 2551 | CA  | LEU | A | 355 | 11.156 | 28.896 | 17.757 | 1.00 | 11.35 | A |
| ATOM | 2552 | CB  | LEU | A | 355 | 12.292 | 28.069 | 17.185 | 1.00 | 12.01 | A |
| ATOM | 2553 | CG  | LEU | A | 355 | 13.697 | 28.633 | 17.424 | 1.00 | 18.77 | A |
| ATOM | 2554 | CD1 | LEU | A | 355 | 14.731 | 27.617 | 16.930 | 1.00 | 13.44 | A |
| ATOM | 2555 | CD2 | LEU | A | 355 | 13.856 | 29.963 | 16.666 | 1.00 | 19.42 | A |
| ATOM | 2556 | C   | LEU | A | 355 | 9.848  | 28.484 | 17.086 | 1.00 | 12.49 | A |
| ATOM | 2557 | O   | LEU | A | 355 | 9.337  | 29.208 | 16.231 | 1.00 | 13.91 | A |
| ATOM | 2558 | N   | THR | A | 356 | 9.300  | 27.331 | 17.458 | 1.00 | 13.88 | A |
| ATOM | 2559 | CA  | THR | A | 356 | 8.036  | 26.866 | 16.849 | 1.00 | 16.44 | A |
| ATOM | 2560 | CB  | THR | A | 356 | 7.414  | 25.759 | 17.704 | 1.00 | 19.06 | A |
| ATOM | 2561 | OG1 | THR | A | 356 | 8.352  | 24.678 | 17.794 | 1.00 | 22.02 | A |
| ATOM | 2562 | CG2 | THR | A | 356 | 6.108  | 25.265 | 17.077 | 1.00 | 20.44 | A |
| ATOM | 2563 | C   | THR | A | 356 | 7.058  | 28.040 | 16.684 | 1.00 | 15.88 | A |
| ATOM | 2564 | O   | THR | A | 356 | 6.609  | 28.642 | 17.658 | 1.00 | 14.53 | A |
| ATOM | 2565 | N   | ALA | A | 357 | 6.720  | 28.362 | 15.441 | 1.00 | 16.53 | A |
| ATOM | 2566 | CA  | ALA | A | 357 | 5.892  | 29.536 | 15.175 | 1.00 | 15.13 | A |
| ATOM | 2567 | CB  | ALA | A | 357 | 5.654  | 29.669 | 13.662 | 1.00 | 17.87 | A |
| ATOM | 2568 | C   | ALA | A | 357 | 4.569  | 29.630 | 15.918 | 1.00 | 18.27 | A |
| ATOM | 2569 | O   | ALA | A | 357 | 4.141  | 30.714 | 16.295 | 1.00 | 19.17 | A |
| ATOM | 2570 | N   | SER | A | 358 | 3.930  | 28.492 | 16.127 | 1.00 | 18.84 | A |
| ATOM | 2571 | CA  | SER | A | 358 | 2.643  | 28.444 | 16.800 | 1.00 | 22.62 | A |
| ATOM | 2572 | CB  | SER | A | 358 | 1.953  | 27.125 | 16.459 | 1.00 | 18.79 | A |
| ATOM | 2573 | OG  | SER | A | 358 | 2.853  | 26.049 | 16.654 | 1.00 | 21.93 | A |
| ATOM | 2574 | C   | SER | A | 358 | 2.716  | 28.607 | 18.318 | 1.00 | 22.54 | A |
| ATOM | 2575 | O   | SER | A | 358 | 1.719  | 28.918 | 18.949 | 1.00 | 19.82 | A |
| ATOM | 2576 | N   | ASN | A | 359 | 3.886  | 28.410 | 18.916 | 1.00 | 20.48 | A |
| ATOM | 2577 | CA  | ASN | A | 359 | 3.950  | 28.550 | 20.358 | 1.00 | 16.65 | A |
| ATOM | 2578 | CB  | ASN | A | 359 | 5.249  | 27.956 | 20.909 | 1.00 | 12.27 | A |
| ATOM | 2579 | CG  | ASN | A | 359 | 5.180  | 27.718 | 22.387 | 1.00 | 11.80 | A |

FIGURE 5 (suite)

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 2580 | OD1 | ASN | A | 359 | 4.992  | 28.652 | 23.170 | 1.00 | 16.11 | A |
| ATOM | 2581 | ND2 | ASN | A | 359 | 5.329  | 26.451 | 22.793 | 1.00 | 14.58 | A |
| ATOM | 2582 | C   | ASN | A | 359 | 3.844  | 30.019 | 20.745 | 1.00 | 16.93 | A |
| ATOM | 2583 | O   | ASN | A | 359 | 4.550  | 30.861 | 20.194 | 1.00 | 15.08 | A |
| ATOM | 2584 | N   | ALA | A | 360 | 2.972  | 30.306 | 21.712 | 1.00 | 15.71 | A |
| ATOM | 2585 | CA  | ALA | A | 360 | 2.759  | 31.664 | 22.208 | 1.00 | 18.67 | A |
| ATOM | 2586 | CB  | ALA | A | 360 | 1.688  | 31.651 | 23.320 | 1.00 | 22.67 | A |
| ATOM | 2587 | C   | ALA | A | 360 | 4.041  | 32.309 | 22.744 | 1.00 | 18.59 | A |
| ATOM | 2588 | O   | ALA | A | 360 | 4.138  | 33.532 | 22.825 | 1.00 | 16.11 | A |
| ATOM | 2589 | N   | LEU | A | 361 | 5.010  | 31.488 | 23.144 | 1.00 | 14.62 | A |
| ATOM | 2590 | CA  | LEU | A | 361 | 6.276  | 32.021 | 23.653 | 1.00 | 11.27 | A |
| ATOM | 2591 | CB  | LEU | A | 361 | 6.863  | 31.060 | 24.685 | 1.00 | 15.51 | A |
| ATOM | 2592 | CG  | LEU | A | 361 | 6.087  | 30.788 | 25.971 | 1.00 | 15.37 | A |
| ATOM | 2593 | CD1 | LEU | A | 361 | 6.713  | 29.586 | 26.688 | 1.00 | 15.50 | A |
| ATOM | 2594 | CD2 | LEU | A | 361 | 6.086  | 32.030 | 26.849 | 1.00 | 14.07 | A |
| ATOM | 2595 | C   | LEU | A | 361 | 7.334  | 32.219 | 22.545 | 1.00 | 12.87 | A |
| ATOM | 2596 | O   | LEU | A | 361 | 8.430  | 32.716 | 22.818 | 1.00 | 12.41 | A |
| ATOM | 2597 | N   | SER | A | 362 | 7.036  | 31.821 | 21.314 | 1.00 | 9.97  | A |
| ATOM | 2598 | CA  | SER | A | 362 | 8.044  | 31.936 | 20.257 | 1.00 | 10.76 | A |
| ATOM | 2599 | CB  | SER | A | 362 | 7.627  | 31.145 | 19.011 | 1.00 | 15.72 | A |
| ATOM | 2600 | OG  | SER | A | 362 | 6.470  | 31.707 | 18.416 | 1.00 | 18.79 | A |
| ATOM | 2601 | C   | SER | A | 362 | 8.454  | 33.338 | 19.822 | 1.00 | 12.29 | A |
| ATOM | 2602 | O   | SER | A | 362 | 7.637  | 34.258 | 19.742 | 1.00 | 12.85 | A |
| ATOM | 2603 | N   | ILE | A | 363 | 9.741  | 33.457 | 19.512 | 1.00 | 10.84 | A |
| ATOM | 2604 | CA  | ILE | A | 363 | 10.353 | 34.698 | 19.072 | 1.00 | 14.99 | A |
| ATOM | 2605 | CB  | ILE | A | 363 | 11.850 | 34.461 | 18.777 | 1.00 | 13.05 | A |
| ATOM | 2606 | CG2 | ILE | A | 363 | 12.483 | 35.713 | 18.198 | 1.00 | 12.46 | A |
| ATOM | 2607 | CG1 | ILE | A | 363 | 12.578 | 34.071 | 20.064 | 1.00 | 15.60 | A |
| ATOM | 2608 | CD1 | ILE | A | 363 | 13.960 | 33.442 | 19.815 | 1.00 | 11.48 | A |
| ATOM | 2609 | C   | ILE | A | 363 | 9.639  | 35.206 | 17.807 | 1.00 | 14.29 | A |
| ATOM | 2610 | O   | ILE | A | 363 | 9.509  | 34.481 | 16.830 | 1.00 | 12.01 | A |
| ATOM | 2611 | N   | GLY | A | 364 | 9.176  | 36.451 | 17.848 | 1.00 | 15.53 | A |
| ATOM | 2612 | CA  | GLY | A | 364 | 8.477  | 37.034 | 16.717 | 1.00 | 14.88 | A |
| ATOM | 2613 | C   | GLY | A | 364 | 7.040  | 36.567 | 16.514 | 1.00 | 19.34 | A |
| ATOM | 2614 | O   | GLY | A | 364 | 6.436  | 36.872 | 15.487 | 1.00 | 19.36 | A |
| ATOM | 2615 | N   | ASP | A | 365 | 6.471  | 35.842 | 17.474 | 1.00 | 15.42 | A |
| ATOM | 2616 | CA  | ASP | A | 365 | 5.094  | 35.360 | 17.323 | 1.00 | 16.08 | A |
| ATOM | 2617 | CB  | ASP | A | 365 | 4.625  | 34.691 | 18.613 | 1.00 | 17.24 | A |
| ATOM | 2618 | CG  | ASP | A | 365 | 3.195  | 34.201 | 18.516 | 1.00 | 22.13 | A |
| ATOM | 2619 | OD1 | ASP | A | 365 | 2.992  | 33.003 | 18.238 | 1.00 | 24.97 | A |
| ATOM | 2620 | OD2 | ASP | A | 365 | 2.272  | 35.025 | 18.698 | 1.00 | 22.46 | A |
| ATOM | 2621 | C   | ASP | A | 365 | 4.100  | 36.490 | 16.954 | 1.00 | 20.12 | A |
| ATOM | 2622 | O   | ASP | A | 365 | 3.979  | 37.482 | 17.668 | 1.00 | 17.92 | A |
| ATOM | 2623 | N   | SER | A | 366 | 3.379  | 36.317 | 15.848 | 1.00 | 21.25 | A |
| ATOM | 2624 | CA  | SER | A | 366 | 2.419  | 37.319 | 15.360 | 1.00 | 19.32 | A |
| ATOM | 2625 | CB  | SER | A | 366 | 1.704  | 36.787 | 14.108 | 1.00 | 21.13 | A |
| ATOM | 2626 | OG  | SER | A | 366 | 2.640  | 36.400 | 13.125 | 1.00 | 29.92 | A |
| ATOM | 2627 | C   | SER | A | 366 | 1.359  | 37.814 | 16.342 | 1.00 | 15.84 | A |
| ATOM | 2628 | O   | SER | A | 366 | 1.155  | 39.010 | 16.461 | 1.00 | 22.39 | A |
| ATOM | 2629 | N   | ALA | A | 367 | 0.655  | 36.920 | 17.024 | 1.00 | 18.40 | A |
| ATOM | 2630 | CA  | ALA | A | 367 | -0.384 | 37.363 | 17.965 | 1.00 | 22.33 | A |
| ATOM | 2631 | CB  | ALA | A | 367 | -1.220 | 36.175 | 18.431 | 1.00 | 19.13 | A |
| ATOM | 2632 | C   | ALA | A | 367 | 0.182  | 38.093 | 19.187 | 1.00 | 25.24 | A |
| ATOM | 2633 | O   | ALA | A | 367 | -0.402 | 39.066 | 19.682 | 1.00 | 26.45 | A |
| ATOM | 2634 | N   | VAL | A | 368 | 1.311  | 37.612 | 19.692 | 1.00 | 24.39 | A |
| ATOM | 2635 | CA  | VAL | A | 368 | 1.903  | 38.229 | 20.864 | 1.00 | 21.43 | A |
| ATOM | 2636 | CB  | VAL | A | 368 | 2.729  | 37.182 | 21.657 | 1.00 | 23.84 | A |
| ATOM | 2637 | CG1 | VAL | A | 368 | 3.447  | 37.838 | 22.850 | 1.00 | 19.42 | A |
| ATOM | 2638 | CG2 | VAL | A | 368 | 1.810  | 36.094 | 22.148 | 1.00 | 25.28 | A |
| ATOM | 2639 | C   | VAL | A | 368 | 2.770  | 39.447 | 20.558 | 1.00 | 19.50 | A |
| ATOM | 2640 | O   | VAL | A | 368 | 2.713  | 40.440 | 21.277 | 1.00 | 22.77 | A |
| ATOM | 2641 | N   | CYS | A | 369 | 3.557  | 39.396 | 19.491 | 1.00 | 17.47 | A |
| ATOM | 2642 | CA  | CYS | A | 369 | 4.448  | 40.505 | 19.195 | 1.00 | 20.32 | A |
| ATOM | 2643 | C   | CYS | A | 369 | 3.919  | 41.648 | 18.322 | 1.00 | 23.64 | A |
| ATOM | 2644 | O   | CYS | A | 369 | 4.617  | 42.639 | 18.120 | 1.00 | 26.98 | A |
| ATOM | 2645 | CB  | CYS | A | 369 | 5.746  | 39.977 | 18.581 | 1.00 | 22.42 | A |
| ATOM | 2646 | SG  | CYS | A | 369 | 6.819  | 38.961 | 19.671 | 1.00 | 19.53 | A |
| ATOM | 2647 | N   | GLY | A | 370 | 2.698  | 41.521 | 17.812 | 1.00 | 25.38 | A |
| ATOM | 2648 | CA  | GLY | A | 370 | 2.154  | 42.575 | 16.966 | 1.00 | 27.80 | A |
| ATOM | 2649 | C   | GLY | A | 370 | 2.190  | 43.938 | 17.627 | 1.00 | 21.46 | A |
| ATOM | 2650 | O   | GLY | A | 370 | 1.631  | 44.112 | 18.705 | 1.00 | 25.76 | A |
| ATOM | 2651 | N   | GLY | A | 371 | 2.872  | 44.885 | 16.988 | 1.00 | 20.44 | A |
| ATOM | 2652 | CA  | GLY | A | 371 | 2.970  | 46.237 | 17.516 | 1.00 | 23.12 | A |
| ATOM | 2653 | C   | GLY | A | 371 | 3.913  | 46.463 | 18.695 | 1.00 | 26.63 | A |
| ATOM | 2654 | O   | GLY | A | 371 | 3.946  | 47.561 | 19.263 | 1.00 | 23.97 | A |
| ATOM | 2655 | N   | LYS | A | 372 | 4.689  | 45.443 | 19.057 | 1.00 | 23.24 | A |

FIGURE 5 (suite)

|      |      |     |     |       |     |        |        |        |      |       |   |
|------|------|-----|-----|-------|-----|--------|--------|--------|------|-------|---|
| ATOM | 2656 | CA  | LYS | A     | 372 | 5.612  | 45.537 | 20.197 | 1.00 | 21.66 | A |
| ATOM | 2657 | CB  | LYS | A     | 372 | 5.141  | 44.605 | 21.296 | 1.00 | 19.20 | A |
| ATOM | 2658 | CG  | LYS | A     | 372 | 3.715  | 44.856 | 21.675 | 1.00 | 25.31 | A |
| ATOM | 2659 | CD  | LYS | A     | 372 | 3.278  | 43.936 | 22.769 | 1.00 | 24.34 | A |
| ATOM | 2660 | CE  | LYS | A     | 372 | 1.884  | 44.315 | 23.208 | 1.00 | 29.63 | A |
| ATOM | 2661 | NZ  | LYS | A     | 372 | 1.426  | 43.423 | 24.285 | 1.00 | 25.95 | A |
| ATOM | 2662 | C   | LYS | A     | 372 | 7.037  | 45.167 | 19.855 | 1.00 | 18.74 | A |
| ATOM | 2663 | O   | LYS | A     | 372 | 7.337  | 44.799 | 18.721 | 1.00 | 17.43 | A |
| ATOM | 2664 | N   | GLY | A     | 373 | 7.917  | 45.247 | 20.852 | 1.00 | 15.44 | A |
| ATOM | 2665 | CA  | GLY | A     | 373 | 9.297  | 44.876 | 20.616 | 1.00 | 12.87 | A |
| ATOM | 2666 | C   | GLY | A     | 373 | 10.366 | 45.876 | 21.015 | 1.00 | 17.42 | A |
| ATOM | 2667 | O   | GLY | A     | 373 | 10.168 | 47.106 | 20.965 | 1.00 | 13.70 | A |
| ATOM | 2668 | N   | ARG | A     | 374 | 11.517 | 45.342 | 21.419 | 1.00 | 14.49 | A |
| ATOM | 2669 | CA  | ARG | A     | 374 | 12.639 | 46.187 | 21.792 | 1.00 | 13.29 | A |
| ATOM | 2670 | CB  | ARG | A     | 374 | 13.786 | 45.339 | 22.333 | 1.00 | 15.72 | A |
| ATOM | 2671 | CG  | ARG | A     | 374 | 13.456 | 44.710 | 23.692 | 1.00 | 18.10 | A |
| ATOM | 2672 | CD  | ARG | A     | 374 | 14.668 | 44.080 | 24.332 | 1.00 | 20.11 | A |
| ATOM | 2673 | NE  | ARG | A     | 374 | 15.729 | 45.034 | 24.665 | 1.00 | 13.47 | A |
| ATOM | 2674 | CZ  | ARG | A     | 374 | 16.143 | 45.296 | 25.699 | 1.00 | 13.50 | A |
| ATOM | 2675 | NH1 | ARG | A     | 374 | 15.564 | 44.694 | 26.928 | 1.00 | 11.14 | A |
| ATOM | 2676 | NH2 | ARG | A     | 374 | 17.206 | 46.082 | 26.100 | 1.00 | 9.65  | A |
| ATOM | 2677 | C   | ARG | A     | 374 | 13.097 | 46.989 | 20.563 | 1.00 | 14.09 | A |
| ATOM | 2678 | O   | ARG | A     | 374 | 13.008 | 46.517 | 19.411 | 1.00 | 13.90 | A |
| ATOM | 2679 | N   | PRO | A     | 375 | 13.575 | 48.225 | 20.797 | 1.00 | 13.52 | A |
| ATOM | 2680 | CD  | PRO | A     | 375 | 13.680 | 48.834 | 22.133 | 1.00 | 12.37 | A |
| ATOM | 2681 | CA  | PRO | A     | 375 | 14.051 | 49.137 | 19.753 | 1.00 | 15.51 | A |
| ATOM | 2682 | CB  | PRO | A     | 375 | 14.304 | 50.445 | 20.516 | 1.00 | 18.56 | A |
| ATOM | 2683 | CG  | PRO | A     | 375 | 14.669 | 49.958 | 21.903 | 1.00 | 16.56 | A |
| ATOM | 2684 | C   | PRO | A     | 375 | 15.282 | 48.622 | 19.017 | 1.00 | 16.94 | A |
| ATOM | 2685 | O   | PRO | A     | 375 | 16.130 | 47.953 | 19.605 | 1.00 | 16.29 | A |
| ATOM | 2686 | N   | GLU | A     | 376 | 15.384 | 48.956 | 17.733 | 1.00 | 14.83 | A |
| ATOM | 2687 | CA  | GLU | A     | 376 | 16.501 | 48.480 | 16.928 | 1.00 | 14.54 | A |
| ATOM | 2688 | CB  | GLU | A     | 376 | 16.191 | 48.638 | 15.429 | 1.00 | 20.94 | A |
| ATOM | 2689 | CG  | GLU | A     | 376 | 15.989 | 50.054 | 14.930 | 1.00 | 25.93 | A |
| ATOM | 2690 | CD  | GLU | A     | 376 | 15.840 | 50.093 | 13.408 | 1.00 | 28.12 | A |
| ATOM | 2691 | OE1 | GLU | A     | 376 | 16.852 | 50.265 | 12.693 | 1.00 | 27.73 | A |
| ATOM | 2692 | OE2 | GLU | A     | 376 | 14.706 | 49.921 | 12.926 | 1.00 | 22.85 | A |
| ATOM | 2693 | C   | GLU | A     | 376 | 17.818 | 49.144 | 17.258 | 1.00 | 15.46 | A |
| ATOM | 2694 | O   | GLU | A     | 376 | 17.779 | 50.308 | 17.715 | 1.00 | 20.34 | A |
| ATOM | 2695 | OXT | GLU | A     | 376 | 18.870 | 48.501 | 17.040 | 1.00 | 17.16 | A |
| ATOM | 2696 | OH2 | WAT | S1500 |     | 35.620 | 33.372 | 34.950 | 1.00 | 7.74  | A |
| ATOM | 2697 | OH2 | WAT | S1501 |     | 26.719 | 26.585 | 54.115 | 1.00 | 13.35 | S |
| ATOM | 2698 | OH2 | WAT | S1502 |     | 32.910 | 38.720 | 42.612 | 1.00 | 11.02 | S |
| ATOM | 2699 | OH2 | WAT | S1503 |     | 25.842 | 40.990 | 19.393 | 1.00 | 10.30 | S |
| ATOM | 2700 | OH2 | WAT | S1504 |     | 47.855 | 24.508 | 32.439 | 1.00 | 11.64 | S |
| ATOM | 2701 | OH2 | WAT | S1505 |     | 37.575 | 38.877 | 30.460 | 1.00 | 13.25 | S |
| ATOM | 2702 | OH2 | WAT | S1506 |     | 43.970 | 19.166 | 36.360 | 1.00 | 11.89 | S |
| ATOM | 2703 | OH2 | WAT | S1507 |     | 51.431 | 26.280 | 38.870 | 1.00 | 11.08 | S |
| ATOM | 2704 | OH2 | WAT | S1508 |     | 21.180 | 34.238 | 33.496 | 1.00 | 10.94 | S |
| ATOM | 2705 | OH2 | WAT | S1509 |     | 34.016 | 23.145 | 55.150 | 1.00 | 7.21  | S |
| ATOM | 2706 | OH2 | WAT | S1510 |     | 34.137 | 35.767 | 50.996 | 1.00 | 14.32 | S |
| ATOM | 2707 | OH2 | WAT | S1511 |     | 29.833 | 31.064 | 61.815 | 1.00 | 12.62 | S |
| ATOM | 2708 | OH2 | WAT | S1512 |     | 36.421 | 34.348 | 51.750 | 1.00 | 8.81  | S |
| ATOM | 2709 | OH2 | WAT | S1513 |     | 24.593 | 22.841 | 22.601 | 1.00 | 14.49 | S |
| ATOM | 2710 | OH2 | WAT | S1514 |     | 33.875 | 20.919 | 53.336 | 1.00 | 15.73 | S |
| ATOM | 2711 | OH2 | WAT | S1515 |     | 55.590 | 18.894 | 44.228 | 1.00 | 20.22 | S |
| ATOM | 2712 | OH2 | WAT | S1516 |     | 25.163 | 24.507 | 19.298 | 1.00 | 7.32  | S |
| ATOM | 2713 | OH2 | WAT | S1517 |     | 29.287 | 27.565 | 53.584 | 1.00 | 10.43 | S |
| ATOM | 2714 | OH2 | WAT | S1518 |     | 27.630 | 35.157 | 54.573 | 1.00 | 11.84 | S |
| ATOM | 2715 | OH2 | WAT | S1519 |     | 34.308 | 40.814 | 45.314 | 1.00 | 9.91  | S |
| ATOM | 2716 | OH2 | WAT | S1520 |     | 24.097 | 26.340 | 47.444 | 1.00 | 12.35 | S |
| ATOM | 2717 | OH2 | WAT | S1521 |     | 26.289 | 17.353 | 26.191 | 1.00 | 14.15 | S |
| ATOM | 2718 | OH2 | WAT | S1522 |     | 31.025 | 26.248 | 57.309 | 1.00 | 9.97  | S |
| ATOM | 2719 | OH2 | WAT | S1523 |     | 16.012 | 33.323 | 36.822 | 1.00 | 10.61 | S |
| ATOM | 2720 | OH2 | WAT | S1524 |     | 35.079 | 31.981 | 26.882 | 1.00 | 7.27  | S |
| ATOM | 2721 | OH2 | WAT | S1525 |     | 48.948 | 16.302 | 35.666 | 1.00 | 22.32 | S |
| ATOM | 2722 | OH2 | WAT | S1526 |     | 23.036 | 32.247 | 50.228 | 1.00 | 12.80 | S |
| ATOM | 2723 | OH2 | WAT | S1527 |     | 41.445 | 42.204 | 48.819 | 1.00 | 16.71 | S |
| ATOM | 2724 | OH2 | WAT | S1528 |     | 30.777 | 34.835 | 16.827 | 1.00 | 12.96 | S |
| ATOM | 2725 | OH2 | WAT | S1529 |     | 9.482  | 33.895 | 27.983 | 1.00 | 10.22 | S |
| ATOM | 2726 | OH2 | WAT | S1530 |     | 10.107 | 31.646 | 29.601 | 1.00 | 12.12 | S |
| ATOM | 2727 | OH2 | WAT | S1531 |     | 37.836 | 31.446 | 58.127 | 1.00 | 18.63 | S |
| ATOM | 2728 | OH2 | WAT | S1532 |     | 23.419 | 29.528 | 35.937 | 1.00 | 10.10 | S |
| ATOM | 2729 | OH2 | WAT | S1533 |     | 36.234 | 16.727 | 51.505 | 1.00 | 9.28  | S |
| ATOM | 2730 | OH2 | WAT | S1534 |     | 5.728  | 38.503 | 24.985 | 1.00 | 13.33 | S |
| ATOM | 2731 | OH2 | WAT | S1535 |     | 29.914 | 14.295 | 35.432 | 1.00 | 16.41 | S |

FIGURE 5 (suite)

|      |      |     |     |       |        |        |        |      |       |   |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|---|
| ATOM | 2732 | OH2 | WAT | S1536 | 31.310 | 38.281 | 18.695 | 1.00 | 9.93  | S |
| ATOM | 2733 | OH2 | WAT | S1537 | 44.863 | 16.606 | 36.022 | 1.00 | 15.09 | S |
| ATOM | 2734 | OH2 | WAT | S1538 | 40.186 | 22.869 | 38.700 | 1.00 | 9.90  | S |
| ATOM | 2735 | OH2 | WAT | S1539 | 37.549 | 20.501 | 28.090 | 1.00 | 13.36 | S |
| ATOM | 2736 | OH2 | WAT | S1540 | 12.913 | 31.829 | 29.436 | 1.00 | 9.36  | S |
| ATOM | 2737 | OH2 | WAT | S1541 | 30.589 | 15.671 | 37.530 | 1.00 | 12.47 | S |
| ATOM | 2738 | OH2 | WAT | S1542 | 23.885 | 35.406 | 43.402 | 1.00 | 18.37 | S |
| ATOM | 2739 | OH2 | WAT | S1543 | 8.663  | 34.010 | 25.289 | 1.00 | 13.37 | S |
| ATOM | 2740 | OH2 | WAT | S1544 | 13.484 | 46.444 | 33.757 | 1.00 | 12.24 | S |
| ATOM | 2741 | OH2 | WAT | S1545 | 27.923 | 19.477 | 57.944 | 1.00 | 11.68 | S |
| ATOM | 2742 | OH2 | WAT | S1546 | 17.540 | 33.345 | 7.715  | 1.00 | 19.22 | S |
| ATOM | 2743 | OH2 | WAT | S1547 | 51.552 | 13.602 | 41.885 | 1.00 | 25.84 | S |
| ATOM | 2744 | OH2 | WAT | S1548 | 27.270 | 26.074 | 40.675 | 1.00 | 10.51 | S |
| ATOM | 2745 | OH2 | WAT | S1549 | 27.760 | 43.771 | 20.816 | 1.00 | 13.46 | S |
| ATOM | 2746 | OH2 | WAT | S1550 | 37.046 | 17.292 | 27.914 | 1.00 | 14.34 | S |
| ATOM | 2747 | OH2 | WAT | S1551 | 37.573 | 33.819 | 20.741 | 1.00 | 23.07 | S |
| ATOM | 2748 | OH2 | WAT | S1552 | 40.930 | 14.067 | 35.565 | 1.00 | 17.08 | S |
| ATOM | 2749 | OH2 | WAT | S1553 | 4.472  | 29.061 | 32.567 | 1.00 | 18.41 | S |
| ATOM | 2750 | OH2 | WAT | S1554 | 26.302 | 32.912 | 28.375 | 1.00 | 10.00 | S |
| ATOM | 2751 | OH2 | WAT | S1555 | 14.165 | 45.737 | 16.934 | 1.00 | 13.06 | S |
| ATOM | 2752 | OH2 | WAT | S1556 | 29.555 | 43.029 | 36.030 | 1.00 | 7.32  | S |
| ATOM | 2753 | OH2 | WAT | S1557 | 36.451 | 34.819 | 37.298 | 1.00 | 11.33 | S |
| ATOM | 2754 | OH2 | WAT | S1558 | 31.931 | 17.255 | 49.603 | 1.00 | 39.16 | S |
| ATOM | 2755 | OH2 | WAT | S1559 | 23.622 | 26.926 | 37.001 | 1.00 | 11.87 | S |
| ATOM | 2756 | OH2 | WAT | S1560 | 31.327 | 13.311 | 33.059 | 1.00 | 12.47 | S |
| ATOM | 2757 | OH2 | WAT | S1561 | 44.899 | 41.787 | 36.741 | 1.00 | 23.25 | S |
| ATOM | 2758 | OH2 | WAT | S1562 | 44.879 | 35.365 | 50.334 | 1.00 | 9.60  | S |
| ATOM | 2759 | OH2 | WAT | S1563 | 20.827 | 50.011 | 18.100 | 1.00 | 15.06 | S |
| ATOM | 2760 | OH2 | WAT | S1564 | 24.374 | 31.041 | 38.304 | 1.00 | 12.38 | S |
| ATOM | 2761 | OH2 | WAT | S1565 | 11.411 | 42.003 | 26.114 | 1.00 | 14.55 | S |
| ATOM | 2762 | OH2 | WAT | S1566 | 21.341 | 35.751 | 40.722 | 1.00 | 12.16 | S |
| ATOM | 2763 | OH2 | WAT | S1567 | 10.175 | 31.393 | 39.888 | 1.00 | 37.76 | S |
| ATOM | 2764 | OH2 | WAT | S1568 | 47.181 | 26.945 | 33.704 | 1.00 | 12.30 | S |
| ATOM | 2765 | OH2 | WAT | S1569 | 42.028 | 43.488 | 36.919 | 1.00 | 25.46 | S |
| ATOM | 2766 | OH2 | WAT | S1570 | 31.053 | 24.724 | 15.706 | 1.00 | 12.46 | S |
| ATOM | 2767 | OH2 | WAT | S1571 | 10.314 | 39.156 | 33.480 | 1.00 | 10.32 | S |
| ATOM | 2768 | OH2 | WAT | S1572 | 51.433 | 20.485 | 50.130 | 1.00 | 15.09 | S |
| ATOM | 2769 | OH2 | WAT | S1573 | 43.925 | 30.656 | 51.790 | 1.00 | 17.28 | S |
| ATOM | 2770 | OH2 | WAT | S1574 | 23.091 | 53.758 | 28.375 | 1.00 | 12.50 | S |
| ATOM | 2771 | OH2 | WAT | S1575 | 34.977 | 41.183 | 53.019 | 1.00 | 15.31 | S |
| ATOM | 2772 | OH2 | WAT | S1576 | 29.766 | 26.781 | 12.309 | 1.00 | 18.82 | S |
| ATOM | 2773 | OH2 | WAT | S1577 | 9.190  | 36.561 | 30.593 | 1.00 | 11.25 | S |
| ATOM | 2774 | OH2 | WAT | S1578 | 36.599 | 15.728 | 48.666 | 1.00 | 21.18 | S |
| ATOM | 2775 | OH2 | WAT | S1579 | 37.724 | 34.865 | 54.143 | 1.00 | 11.62 | S |
| ATOM | 2776 | OH2 | WAT | S1580 | 21.457 | 35.713 | 12.303 | 1.00 | 13.24 | S |
| ATOM | 2777 | OH2 | WAT | S1581 | 27.734 | 31.073 | 59.797 | 1.00 | 14.78 | S |
| ATOM | 2778 | OH2 | WAT | S1582 | 51.536 | 35.554 | 40.163 | 1.00 | 14.52 | S |
| ATOM | 2779 | OH2 | WAT | S1583 | 29.933 | 42.651 | 53.057 | 1.00 | 14.55 | S |
| ATOM | 2780 | OH2 | WAT | S1584 | 9.469  | 23.677 | 25.125 | 1.00 | 12.14 | S |
| ATOM | 2781 | OH2 | WAT | S1585 | 20.704 | 29.372 | 11.334 | 1.00 | 17.80 | S |
| ATOM | 2782 | OH2 | WAT | S1586 | 56.481 | 22.975 | 38.435 | 1.00 | 29.16 | S |
| ATOM | 2783 | OH2 | WAT | S1587 | 9.572  | 40.421 | 17.037 | 1.00 | 14.99 | S |
| ATOM | 2784 | OH2 | WAT | S1588 | 20.542 | 42.224 | 40.862 | 1.00 | 13.90 | S |
| ATOM | 2785 | OH2 | WAT | S1589 | 9.567  | 37.848 | 39.841 | 1.00 | 15.10 | S |
| ATOM | 2786 | OH2 | WAT | S1590 | 6.391  | 48.835 | 28.636 | 1.00 | 19.52 | S |
| ATOM | 2787 | OH2 | WAT | S1591 | 41.492 | 20.894 | 55.469 | 1.00 | 16.40 | S |
| ATOM | 2788 | OH2 | WAT | S1592 | 22.505 | 28.556 | 52.952 | 1.00 | 24.23 | S |
| ATOM | 2789 | OH2 | WAT | S1593 | 27.720 | 46.441 | 20.204 | 1.00 | 15.40 | S |
| ATOM | 2790 | OH2 | WAT | S1594 | 37.216 | 41.499 | 30.864 | 1.00 | 19.68 | S |
| ATOM | 2791 | OH2 | WAT | S1595 | 30.199 | 27.159 | 15.034 | 1.00 | 11.19 | S |
| ATOM | 2792 | OH2 | WAT | S1596 | 25.139 | 30.964 | 53.858 | 1.00 | 21.47 | S |
| ATOM | 2793 | OH2 | WAT | S1597 | 35.730 | 20.698 | 18.767 | 1.00 | 15.15 | S |
| ATOM | 2794 | OH2 | WAT | S1598 | 44.994 | 20.666 | 23.797 | 1.00 | 17.67 | S |
| ATOM | 2795 | OH2 | WAT | S1599 | 28.802 | 58.069 | 26.514 | 1.00 | 17.28 | S |
| ATOM | 2796 | OH2 | WAT | S1600 | 16.767 | 47.104 | 22.319 | 1.00 | 11.98 | S |
| ATOM | 2797 | OH2 | WAT | S1601 | 30.159 | 33.756 | 60.797 | 1.00 | 9.19  | S |
| ATOM | 2798 | OH2 | WAT | S1602 | 48.106 | 27.997 | 36.005 | 1.00 | 14.93 | S |
| ATOM | 2799 | OH2 | WAT | S1603 | 40.650 | 24.407 | 21.552 | 1.00 | 17.12 | S |
| ATOM | 2800 | OH2 | WAT | S1604 | 22.968 | 17.449 | 18.008 | 1.00 | 17.85 | S |
| ATOM | 2801 | OH2 | WAT | S1605 | 16.621 | 15.788 | 18.605 | 1.00 | 25.68 | S |
| ATOM | 2802 | OH2 | WAT | S1606 | 7.206  | 32.992 | 16.005 | 1.00 | 14.53 | S |
| ATOM | 2803 | OH2 | WAT | S1607 | 57.149 | 24.564 | 47.629 | 1.00 | 18.35 | S |
| ATOM | 2804 | OH2 | WAT | S1608 | 24.205 | 26.840 | 10.350 | 1.00 | 23.21 | S |
| ATOM | 2805 | OH2 | WAT | S1609 | 33.745 | 22.604 | 31.364 | 1.00 | 14.24 | S |
| ATOM | 2806 | OH2 | WAT | S1610 | 21.687 | 28.608 | 49.750 | 1.00 | 41.13 | S |
| ATOM | 2807 | OH2 | WAT | S1611 | 25.572 | 18.289 | 18.085 | 1.00 | 18.47 | S |

FIGURE 5 (suite)

|      |      |     |     |       |        |        |        |      |       |   |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|---|
| ATOM | 2808 | OH2 | WAT | S1612 | 29.378 | 22.049 | 15.378 | 1.00 | 18.53 | S |
| ATOM | 2809 | OH2 | WAT | S1613 | 47.580 | 17.180 | 46.156 | 1.00 | 18.00 | S |
| ATOM | 2810 | OH2 | WAT | S1614 | 23.216 | 43.309 | 37.644 | 1.00 | 13.17 | S |
| ATOM | 2811 | OH2 | WAT | S1615 | 22.669 | 24.274 | 48.564 | 1.00 | 24.15 | S |
| ATOM | 2812 | OH2 | WAT | S1616 | 0.336  | 31.433 | 18.582 | 1.00 | 27.87 | S |
| ATOM | 2813 | OH2 | WAT | S1617 | 45.294 | 33.053 | 51.773 | 1.00 | 13.88 | S |
| ATOM | 2814 | OH2 | WAT | S1618 | 44.363 | 26.868 | 22.624 | 1.00 | 23.01 | S |
| ATOM | 2815 | OH2 | WAT | S1619 | 24.023 | 16.291 | 14.532 | 1.00 | 14.28 | S |
| ATOM | 2816 | OH2 | WAT | S1620 | 25.803 | 16.259 | 28.626 | 1.00 | 18.77 | S |
| ATOM | 2817 | OH2 | WAT | S1621 | 10.423 | 51.944 | 32.078 | 1.00 | 36.29 | S |
| ATOM | 2818 | OH2 | WAT | S1622 | 26.115 | 58.809 | 27.014 | 1.00 | 15.64 | S |
| ATOM | 2819 | OH2 | WAT | S1623 | 1.344  | 28.356 | 22.672 | 1.00 | 26.37 | S |
| ATOM | 2820 | OH2 | WAT | S1624 | 26.639 | 58.198 | 21.115 | 1.00 | 25.02 | S |
| ATOM | 2821 | OH2 | WAT | S1625 | 26.622 | 32.997 | 55.284 | 1.00 | 16.24 | S |
| ATOM | 2822 | OH2 | WAT | S1626 | 15.027 | 52.473 | 26.183 | 1.00 | 21.76 | S |
| ATOM | 2823 | OH2 | WAT | S1627 | 57.187 | 25.783 | 44.900 | 1.00 | 20.20 | S |
| ATOM | 2824 | OH2 | WAT | S1628 | 44.922 | 43.322 | 47.514 | 1.00 | 18.96 | S |
| ATOM | 2825 | OH2 | WAT | S1629 | 32.001 | 38.779 | 53.199 | 1.00 | 17.42 | S |
| ATOM | 2826 | OH2 | WAT | S1630 | 30.741 | 52.390 | 22.108 | 1.00 | 18.11 | S |
| ATOM | 2827 | OH2 | WAT | S1631 | 14.999 | 39.258 | 44.162 | 1.00 | 19.15 | S |
| ATOM | 2828 | OH2 | WAT | S1632 | 44.210 | 20.606 | 55.552 | 1.00 | 17.79 | S |
| ATOM | 2829 | OH2 | WAT | S1633 | 21.471 | 43.377 | 12.416 | 1.00 | 19.05 | S |
| ATOM | 2830 | OH2 | WAT | S1634 | 13.869 | 15.823 | 31.777 | 1.00 | 25.21 | S |
| ATOM | 2831 | OH2 | WAT | S1635 | 52.620 | 30.612 | 55.173 | 1.00 | 30.08 | S |
| ATOM | 2832 | OH2 | WAT | S1636 | 26.556 | 19.486 | 52.050 | 1.00 | 29.07 | S |
| ATOM | 2833 | OH2 | WAT | S1637 | 21.965 | 25.980 | 45.841 | 1.00 | 19.07 | S |
| ATOM | 2834 | OH2 | WAT | S1638 | 51.617 | 33.897 | 42.473 | 1.00 | 9.81  | S |
| ATOM | 2835 | OH2 | WAT | S1639 | 11.552 | 20.655 | 19.351 | 1.00 | 16.68 | S |
| ATOM | 2836 | OH2 | WAT | S1640 | 30.899 | 45.201 | 19.222 | 1.00 | 26.19 | S |
| ATOM | 2837 | OH2 | WAT | S1641 | 31.709 | 48.342 | 31.000 | 1.00 | 18.10 | S |
| ATOM | 2838 | OH2 | WAT | S1642 | 23.676 | 25.327 | 22.818 | 1.00 | 14.28 | S |
| ATOM | 2839 | OH2 | WAT | S1643 | 25.577 | 17.219 | 46.479 | 1.00 | 20.91 | S |
| ATOM | 2840 | OH2 | WAT | S1644 | 18.005 | 18.283 | 19.152 | 1.00 | 24.14 | S |
| ATOM | 2841 | OH2 | WAT | S1645 | 52.881 | 16.705 | 50.095 | 1.00 | 20.16 | S |
| ATOM | 2842 | OH2 | WAT | S1646 | 5.848  | 42.562 | 37.856 | 1.00 | 19.01 | S |
| ATOM | 2843 | OH2 | WAT | S1647 | 43.582 | 14.659 | 34.565 | 1.00 | 28.17 | S |
| ATOM | 2844 | OH2 | WAT | S1648 | 22.374 | 17.743 | 20.886 | 1.00 | 18.81 | S |
| ATOM | 2845 | OH2 | WAT | S1649 | 8.712  | 48.989 | 27.030 | 1.00 | 23.87 | S |
| ATOM | 2846 | OH2 | WAT | S1650 | 2.521  | 47.157 | 34.228 | 1.00 | 30.10 | S |
| ATOM | 2847 | OH2 | WAT | S1651 | 44.220 | 43.064 | 40.109 | 1.00 | 29.97 | S |
| ATOM | 2848 | OH2 | WAT | S1652 | 27.919 | 24.353 | 12.179 | 1.00 | 16.62 | S |
| ATOM | 2849 | OH2 | WAT | S1653 | 3.523  | 42.077 | 26.249 | 1.00 | 22.83 | S |
| ATOM | 2850 | OH2 | WAT | S1654 | 20.380 | 44.291 | 37.672 | 1.00 | 17.30 | S |
| ATOM | 2851 | OH2 | WAT | S1655 | 57.034 | 28.423 | 45.056 | 1.00 | 27.44 | S |
| ATOM | 2852 | OH2 | WAT | S1656 | 49.668 | 24.467 | 30.455 | 1.00 | 22.73 | S |
| ATOM | 2853 | OH2 | WAT | S1657 | 51.259 | 13.409 | 45.586 | 1.00 | 34.23 | S |
| ATOM | 2854 | OH2 | WAT | S1658 | 9.456  | 23.136 | 36.163 | 1.00 | 24.71 | S |
| ATOM | 2855 | OH2 | WAT | S1659 | 52.331 | 23.665 | 57.905 | 1.00 | 18.92 | S |
| ATOM | 2856 | OH2 | WAT | S1660 | 43.381 | 40.535 | 56.268 | 1.00 | 30.03 | S |
| ATOM | 2857 | OH2 | WAT | S1661 | 13.806 | 46.776 | 43.159 | 1.00 | 30.72 | S |
| ATOM | 2858 | OH2 | WAT | S1662 | 53.981 | 30.491 | 48.223 | 1.00 | 13.32 | S |
| ATOM | 2859 | OH2 | WAT | S1663 | 41.765 | 26.570 | 28.744 | 1.00 | 27.76 | S |
| ATOM | 2860 | OH2 | WAT | S1664 | 40.737 | 17.318 | 53.732 | 1.00 | 24.67 | S |
| ATOM | 2861 | OH2 | WAT | S1665 | 13.225 | 44.990 | 8.674  | 1.00 | 28.84 | S |
| ATOM | 2862 | OH2 | WAT | S1666 | 49.013 | 41.254 | 39.651 | 1.00 | 28.00 | S |
| ATOM | 2863 | OH2 | WAT | S1667 | 44.805 | 37.426 | 30.933 | 1.00 | 16.56 | S |
| ATOM | 2864 | OH2 | WAT | S1668 | 43.625 | 18.020 | 54.500 | 1.00 | 24.62 | S |
| ATOM | 2865 | OH2 | WAT | S1669 | 14.317 | 25.699 | 46.118 | 1.00 | 34.64 | S |
| ATOM | 2866 | OH2 | WAT | S1670 | 3.256  | 42.913 | 32.109 | 1.00 | 29.06 | S |
| ATOM | 2867 | OH2 | WAT | S1671 | 10.555 | 49.763 | 20.725 | 1.00 | 28.19 | S |
| ATOM | 2868 | OH2 | WAT | S1672 | 10.096 | 51.223 | 27.611 | 1.00 | 23.49 | S |
| ATOM | 2869 | OH2 | WAT | S1673 | 14.363 | 23.946 | 36.209 | 1.00 | 40.49 | S |
| ATOM | 2870 | OH2 | WAT | S1674 | 25.126 | 59.432 | 22.831 | 1.00 | 22.37 | S |
| ATOM | 2871 | OH2 | WAT | S1675 | 36.093 | 4.004  | 46.425 | 1.00 | 41.05 | S |
| ATOM | 2872 | OH2 | WAT | S1676 | 58.346 | 33.177 | 43.906 | 1.00 | 32.25 | S |
| ATOM | 2873 | OH2 | WAT | S1677 | 48.932 | 35.192 | 51.801 | 1.00 | 26.68 | S |
| ATOM | 2874 | OH2 | WAT | S1678 | 58.902 | 19.301 | 43.107 | 1.00 | 25.48 | S |
| ATOM | 2875 | OH2 | WAT | S1679 | 44.340 | 42.085 | 50.822 | 1.00 | 28.00 | S |
| ATOM | 2876 | OH2 | WAT | S1680 | 50.480 | 38.266 | 34.016 | 1.00 | 31.92 | S |
| ATOM | 2877 | OH2 | WAT | S1681 | 32.259 | 20.178 | 55.706 | 1.00 | 22.68 | S |
| ATOM | 2878 | OH2 | WAT | S1682 | 5.907  | 48.823 | 21.778 | 1.00 | 41.37 | S |
| ATOM | 2879 | OH2 | WAT | S1683 | 50.286 | 29.738 | 36.205 | 1.00 | 41.24 | S |
| ATOM | 2880 | OH2 | WAT | S1684 | 48.359 | 24.392 | 27.682 | 1.00 | 21.59 | S |
| ATOM | 2881 | OH2 | WAT | S1685 | 28.819 | 16.491 | 25.944 | 1.00 | 22.91 | S |
| ATOM | 2882 | OH2 | WAT | S1686 | 27.814 | 39.366 | 53.598 | 1.00 | 22.13 | S |
| ATOM | 2883 | OH2 | WAT | S1687 | 23.282 | 56.182 | 29.647 | 1.00 | 21.73 | S |

FIGURE 5 (suite)

|      |      |     |     |       |        |        |        |      |       |   |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|---|
| ATOM | 2884 | OH2 | WAT | S1688 | 11.176 | 51.488 | 23.245 | 1.00 | 39.40 | S |
| ATOM | 2885 | OH2 | WAT | S1689 | 19.333 | 13.893 | 25.470 | 1.00 | 16.29 | S |
| ATOM | 2886 | OH2 | WAT | S1690 | 15.528 | 35.966 | 43.442 | 1.00 | 24.55 | S |
| ATOM | 2887 | OH2 | WAT | S1691 | 28.485 | 18.098 | 54.189 | 1.00 | 38.82 | S |
| ATOM | 2888 | OH2 | WAT | S1692 | 49.461 | 42.346 | 42.415 | 1.00 | 29.71 | S |
| ATOM | 2889 | OH2 | WAT | S1693 | 6.986  | 51.318 | 31.491 | 1.00 | 38.19 | S |
| ATOM | 2890 | OH2 | WAT | S1694 | 45.805 | 30.330 | 30.352 | 1.00 | 31.74 | S |
| ATOM | 2891 | OH2 | WAT | S1695 | 12.688 | 17.949 | 24.810 | 1.00 | 24.29 | S |
| ATOM | 2892 | OH2 | WAT | S1696 | 10.481 | 44.192 | 41.405 | 1.00 | 30.36 | S |
| ATOM | 2893 | OH2 | WAT | S1697 | 36.497 | 25.163 | 61.042 | 1.00 | 22.75 | S |
| ATOM | 2894 | OH2 | WAT | S1698 | 38.997 | 8.895  | 40.582 | 1.00 | 35.83 | S |
| ATOM | 2895 | OH2 | WAT | S1699 | 34.429 | 41.271 | 24.603 | 1.00 | 25.66 | S |
| ATOM | 2896 | OH2 | WAT | S1700 | 9.264  | 39.356 | 31.031 | 1.00 | 12.79 | S |
| ATOM | 2897 | OH2 | WAT | S1701 | 10.070 | 23.977 | 42.971 | 1.00 | 38.68 | S |
| ATOM | 2898 | OH2 | WAT | S1702 | 18.383 | 29.372 | 9.706  | 1.00 | 35.59 | S |
| ATOM | 2899 | OH2 | WAT | S1703 | 49.044 | 14.511 | 44.663 | 1.00 | 29.13 | S |
| ATOM | 2900 | OH2 | WAT | S1704 | 24.559 | 26.271 | 39.612 | 1.00 | 9.57  | S |
| ATOM | 2901 | OH2 | WAT | S1705 | 20.114 | 45.757 | 12.779 | 1.00 | 24.18 | S |
| ATOM | 2902 | OH2 | WAT | S1706 | 40.248 | 22.113 | 20.074 | 1.00 | 29.44 | S |
| ATOM | 2903 | OH2 | WAT | S1707 | 18.194 | 41.869 | 42.229 | 1.00 | 17.46 | S |
| ATOM | 2904 | OH2 | WAT | S1708 | 37.847 | 20.546 | 20.498 | 1.00 | 18.73 | S |
| ATOM | 2905 | OH2 | WAT | S1709 | 16.821 | 29.280 | 41.001 | 1.00 | 24.06 | S |
| ATOM | 2906 | OH2 | WAT | S1710 | 27.294 | 42.193 | 52.815 | 1.00 | 19.46 | S |
| ATOM | 2907 | OH2 | WAT | S1711 | 40.821 | 42.347 | 51.556 | 1.00 | 22.66 | S |
| ATOM | 2908 | OH2 | WAT | S1712 | 26.156 | 40.106 | 48.095 | 1.00 | 24.85 | S |
| ATOM | 2909 | OH2 | WAT | S1713 | 20.103 | 24.718 | 47.608 | 1.00 | 30.63 | S |
| ATOM | 2910 | OH2 | WAT | S1714 | 24.148 | 33.741 | 56.397 | 1.00 | 19.34 | S |
| ATOM | 2911 | OH2 | WAT | S1715 | 18.973 | 45.993 | 36.285 | 1.00 | 18.68 | S |
| ATOM | 2912 | OH2 | WAT | S1716 | 14.529 | 44.714 | 35.623 | 1.00 | 11.98 | S |
| ATOM | 2913 | OH2 | WAT | S1717 | 38.781 | 35.753 | 22.003 | 1.00 | 28.14 | S |
| ATOM | 2914 | OH2 | WAT | S1718 | 9.031  | 37.190 | 34.220 | 1.00 | 30.97 | S |
| ATOM | 2915 | OH2 | WAT | S1719 | 35.994 | 16.311 | 25.745 | 1.00 | 28.93 | S |
| ATOM | 2916 | OH2 | WAT | S1720 | 13.544 | 49.140 | 34.673 | 1.00 | 19.62 | S |
| ATOM | 2917 | OH2 | WAT | S1721 | 22.265 | 37.832 | 42.637 | 1.00 | 21.65 | S |
| ATOM | 2918 | OH2 | WAT | S1722 | 9.246  | 42.739 | 13.991 | 1.00 | 23.76 | S |
| ATOM | 2919 | OH2 | WAT | S1723 | 46.901 | 14.013 | 46.528 | 1.00 | 24.08 | S |
| ATOM | 2920 | OH2 | WAT | S1724 | 27.124 | 17.124 | 56.373 | 1.00 | 20.76 | S |
| ATOM | 2921 | OH2 | WAT | S1725 | 5.808  | 39.927 | 37.880 | 1.00 | 30.10 | S |
| ATOM | 2922 | OH2 | WAT | S1726 | 42.361 | 20.811 | 20.431 | 1.00 | 24.61 | S |
| ATOM | 2923 | OH2 | WAT | S1727 | 26.665 | 17.537 | 21.374 | 1.00 | 22.27 | S |
| ATOM | 2924 | OH2 | WAT | S1728 | 57.473 | 29.684 | 48.797 | 1.00 | 33.94 | S |
| ATOM | 2925 | OH2 | WAT | S1729 | 0.205  | 29.580 | 11.300 | 1.00 | 28.38 | S |
| ATOM | 2926 | OH2 | WAT | S1730 | 28.982 | 12.144 | 36.663 | 1.00 | 22.16 | S |
| ATOM | 2927 | OH2 | WAT | S1731 | -2.247 | 31.885 | 18.386 | 1.00 | 37.56 | S |
| ATOM | 2928 | OH2 | WAT | S1732 | 19.593 | 14.821 | 28.910 | 1.00 | 29.82 | S |
| ATOM | 2929 | OH2 | WAT | S1733 | 1.174  | 27.052 | 34.363 | 1.00 | 22.10 | S |
| ATOM | 2930 | OH2 | WAT | S1734 | 35.909 | 11.924 | 47.248 | 1.00 | 27.93 | S |
| ATOM | 2931 | OH2 | WAT | S1735 | 41.887 | 40.436 | 52.838 | 1.00 | 28.22 | S |
| ATOM | 2932 | OH2 | WAT | S1736 | 26.213 | 19.454 | 10.997 | 1.00 | 22.64 | S |
| ATOM | 2933 | OH2 | WAT | S1737 | 34.114 | 42.884 | 34.175 | 1.00 | 28.42 | S |
| ATOM | 2934 | OH2 | WAT | S1738 | 22.945 | 32.302 | 53.065 | 1.00 | 25.85 | S |
| ATOM | 2935 | OH2 | WAT | S1739 | 39.089 | 15.172 | 28.466 | 1.00 | 31.20 | S |
| ATOM | 2936 | OH2 | WAT | S1740 | 47.610 | 43.601 | 46.621 | 1.00 | 36.15 | S |
| ATOM | 2937 | OH2 | WAT | S1741 | 16.327 | 45.853 | 37.179 | 1.00 | 17.39 | S |
| ATOM | 2938 | OH2 | WAT | S1742 | 55.363 | 25.260 | 59.367 | 1.00 | 29.21 | S |
| ATOM | 2939 | OH2 | WAT | S1743 | 30.641 | 36.731 | 14.630 | 1.00 | 26.83 | S |
| ATOM | 2940 | OH2 | WAT | S1744 | 10.864 | 46.250 | 10.531 | 1.00 | 23.96 | S |
| ATOM | 2941 | OH2 | WAT | S1745 | 33.170 | 48.399 | 28.312 | 1.00 | 27.45 | S |
| ATOM | 2942 | OH2 | WAT | S1746 | 32.054 | 14.892 | 42.067 | 1.00 | 24.32 | S |
| ATOM | 2943 | OH2 | WAT | S1747 | 42.724 | 28.782 | 21.018 | 1.00 | 34.32 | S |
| ATOM | 2944 | OH2 | WAT | S1748 | 51.123 | 15.697 | 52.194 | 1.00 | 27.97 | S |
| ATOM | 2945 | OH2 | WAT | S1749 | 42.354 | 43.166 | 56.140 | 1.00 | 29.49 | S |
| ATOM | 2946 | OH2 | WAT | S1750 | 28.037 | 37.891 | 13.736 | 1.00 | 33.67 | S |
| ATOM | 2947 | OH2 | WAT | S1751 | 51.086 | 26.646 | 30.768 | 1.00 | 30.84 | S |
| ATOM | 2948 | OH2 | WAT | S1752 | 10.931 | 38.592 | 10.467 | 1.00 | 25.71 | S |
| ATOM | 2949 | OH2 | WAT | S1753 | 25.655 | 29.886 | 60.929 | 1.00 | 19.64 | S |
| ATOM | 2950 | OH2 | WAT | S1754 | 17.145 | 13.376 | 23.383 | 1.00 | 34.23 | S |
| ATOM | 2951 | OH2 | WAT | S1755 | 44.748 | 12.372 | 45.391 | 1.00 | 18.99 | S |
| ATOM | 2952 | OH2 | WAT | S1756 | 24.658 | 10.868 | 33.101 | 1.00 | 39.56 | S |
| ATOM | 2953 | OH2 | WAT | S1757 | 10.322 | 35.265 | 39.792 | 1.00 | 31.55 | S |
| ATOM | 2954 | OH2 | WAT | S1758 | 57.341 | 22.537 | 45.377 | 1.00 | 16.36 | S |
| ATOM | 2955 | OH2 | WAT | S1759 | 9.420  | 34.820 | 36.963 | 1.00 | 32.92 | S |
| ATOM | 2956 | OH2 | WAT | S1760 | 32.502 | 28.596 | 14.854 | 1.00 | 21.37 | S |
| ATOM | 2957 | OH2 | WAT | S1761 | 39.205 | 22.929 | 17.441 | 1.00 | 35.60 | S |
| ATOM | 2958 | OH2 | WAT | S1762 | 20.840 | 52.812 | 17.278 | 1.00 | 31.30 | S |
| ATOM | 2959 | OH2 | WAT | S1763 | 34.711 | 11.735 | 35.138 | 1.00 | 32.11 | S |

FIGURE 5 (suite)

|      |      |     |     |       |        |        |        |      |       |   |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|---|
| ATOM | 2960 | OH2 | WAT | S1764 | 51.666 | 34.131 | 47.365 | 1.00 | 35.34 | S |
| ATOM | 2961 | OH2 | WAT | S1765 | -2.014 | 36.180 | 15.830 | 1.00 | 28.16 | S |
| ATOM | 2962 | OH2 | WAT | S1766 | 15.482 | 48.721 | 37.060 | 1.00 | 29.26 | S |
| ATOM | 2963 | OH2 | WAT | S1767 | 40.630 | 14.716 | 31.062 | 1.00 | 40.40 | S |
| ATOM | 2964 | OH2 | WAT | S1768 | 23.698 | 61.256 | 21.533 | 1.00 | 16.86 | S |
| ATOM | 2965 | OH2 | WAT | S1769 | 24.781 | 28.532 | 54.977 | 1.00 | 16.20 | S |
| ATOM | 2966 | OH2 | WAT | S1770 | 26.852 | 25.257 | 10.061 | 1.00 | 30.41 | S |
| ATOM | 2967 | OH2 | WAT | S1771 | 43.726 | 10.405 | 46.878 | 1.00 | 29.13 | S |
| ATOM | 2968 | OH2 | WAT | S1772 | 25.837 | 37.362 | 54.027 | 1.00 | 21.97 | S |
| ATOM | 2969 | OH2 | WAT | S1773 | 33.373 | 46.686 | 32.566 | 1.00 | 26.20 | S |
| ATOM | 2970 | OH2 | WAT | S1774 | 27.264 | 20.817 | 13.545 | 1.00 | 22.02 | S |
| ATOM | 2971 | OH2 | WAT | S1775 | 47.925 | 30.806 | 31.477 | 1.00 | 33.49 | S |
| ATOM | 2972 | OH2 | WAT | S1776 | 8.238  | 38.202 | 37.592 | 1.00 | 26.28 | S |
| ATOM | 2973 | OH2 | WAT | S1777 | 21.090 | 51.641 | 25.222 | 1.00 | 18.54 | S |
| ATOM | 2974 | OH2 | WAT | S1778 | 6.267  | 38.069 | 32.873 | 1.00 | 22.17 | S |
| ATOM | 2975 | OH2 | WAT | S1779 | 23.234 | 49.347 | 16.745 | 1.00 | 24.08 | S |
| ATOM | 2976 | OH2 | WAT | S1780 | 22.134 | 39.856 | 40.656 | 1.00 | 21.00 | S |
| ATOM | 2977 | OH2 | WAT | S1781 | 20.856 | 35.405 | 9.637  | 1.00 | 23.13 | S |
| ATOM | 2978 | OH2 | WAT | S1782 | 21.475 | 53.999 | 26.047 | 1.00 | 27.01 | S |
| ATOM | 2979 | OH2 | WAT | S1783 | 34.915 | 27.212 | 15.190 | 1.00 | 31.71 | S |
| ATOM | 2980 | OH2 | WAT | S1784 | 45.211 | 12.993 | 42.137 | 1.00 | 21.38 | S |
| ATOM | 2981 | OH2 | WAT | S1785 | 38.126 | 34.805 | 40.034 | 1.00 | 17.57 | S |
| ATOM | 2982 | OH2 | WAT | S1786 | 30.962 | 49.798 | 21.332 | 1.00 | 32.31 | S |
| ATOM | 2983 | OH2 | WAT | S1787 | 33.222 | 19.319 | 25.705 | 1.00 | 29.22 | S |
| ATOM | 2984 | OH2 | WAT | S1788 | 40.144 | 19.662 | 28.253 | 1.00 | 33.93 | S |
| ATOM | 2985 | OH2 | WAT | S1789 | 6.555  | 28.590 | 37.281 | 1.00 | 28.90 | S |
| ATOM | 2986 | OH2 | WAT | S1790 | 43.426 | 43.935 | 45.155 | 1.00 | 34.35 | S |
| ATOM | 2987 | OH2 | WAT | S1791 | 3.263  | 33.201 | 14.705 | 1.00 | 33.11 | S |
| ATOM | 2988 | OH2 | WAT | S1792 | 20.149 | 16.998 | 31.047 | 1.00 | 26.99 | S |
| ATOM | 2989 | OH2 | WAT | S1793 | 34.123 | 42.842 | 21.180 | 1.00 | 24.49 | S |
| ATOM | 2990 | OH2 | WAT | S1794 | 49.929 | 18.274 | 53.829 | 1.00 | 39.26 | S |
| ATOM | 2991 | OH2 | WAT | S1795 | 14.815 | 31.617 | 9.739  | 1.00 | 35.94 | S |
| ATOM | 2992 | OH2 | WAT | S1796 | 45.588 | 41.539 | 53.753 | 1.00 | 35.01 | S |
| ATOM | 2993 | OH2 | WAT | S1797 | 33.245 | 52.433 | 24.002 | 1.00 | 34.85 | S |
| ATOM | 2994 | OH2 | WAT | S1798 | 43.010 | 24.276 | 22.909 | 1.00 | 21.38 | S |
| ATOM | 2995 | OH2 | WAT | S1799 | 19.769 | 14.826 | 46.718 | 1.00 | 30.67 | S |
| ATOM | 2996 | OH2 | WAT | S1800 | 29.812 | 17.873 | 43.458 | 1.00 | 28.85 | S |
| ATOM | 2997 | OH2 | WAT | S1801 | 7.028  | 22.438 | 24.718 | 1.00 | 30.13 | S |
| ATOM | 2998 | OH2 | WAT | S1802 | 7.451  | 42.723 | 16.836 | 1.00 | 34.86 | S |
| ATOM | 2999 | OH2 | WAT | S1803 | 13.062 | 50.532 | 16.899 | 1.00 | 27.23 | S |
| ATOM | 3000 | OH2 | WAT | S1804 | 31.535 | 17.528 | 46.115 | 1.00 | 21.48 | S |
| ATOM | 3001 | OH2 | WAT | S1805 | 1.214  | 41.199 | 23.409 | 1.00 | 33.03 | S |
| ATOM | 3002 | OH2 | WAT | S1806 | 12.350 | 33.958 | 40.836 | 1.00 | 34.82 | S |
| ATOM | 3003 | OH2 | WAT | S1807 | 33.164 | 41.928 | 54.755 | 1.00 | 33.81 | S |
| ATOM | 3004 | OH2 | WAT | S1808 | 4.467  | 50.285 | 27.482 | 1.00 | 36.79 | S |
| ATOM | 3005 | OH2 | WAT | S1809 | 60.702 | 26.732 | 42.684 | 1.00 | 35.13 | S |
| ATOM | 3006 | OH2 | WAT | S1810 | 22.799 | 31.560 | 57.795 | 1.00 | 32.80 | S |
| ATOM | 3007 | OH2 | WAT | S1811 | 16.630 | 35.862 | 8.507  | 1.00 | 29.92 | S |
| ATOM | 3008 | OH2 | WAT | S1812 | 58.212 | 35.487 | 40.540 | 1.00 | 33.76 | S |
| ATOM | 3009 | OH2 | WAT | S1813 | 31.566 | 17.525 | 26.426 | 1.00 | 39.01 | S |
| ATOM | 3010 | OH2 | WAT | S1814 | 38.884 | 37.614 | 20.120 | 1.00 | 33.89 | S |
| ATOM | 3011 | OH2 | WAT | S1815 | 58.154 | 24.777 | 37.822 | 1.00 | 35.73 | S |
| ATOM | 3012 | OH2 | WAT | S1816 | 34.384 | 14.783 | 47.649 | 1.00 | 37.28 | S |
| ATOM | 3013 | OH2 | WAT | S1817 | 3.439  | 43.153 | 36.372 | 1.00 | 30.78 | S |
| ATOM | 3014 | OH2 | WAT | S1818 | 47.394 | 12.444 | 43.290 | 1.00 | 30.32 | S |
| ATOM | 3015 | OH2 | WAT | S1819 | 24.644 | 13.829 | 44.044 | 1.00 | 32.65 | S |
| ATOM | 3016 | OH2 | WAT | S1820 | 35.990 | 42.985 | 32.322 | 1.00 | 29.66 | S |
| ATOM | 3017 | OH2 | WAT | S1821 | 26.914 | 40.212 | 9.947  | 1.00 | 33.58 | S |
| ATOM | 3018 | OH2 | WAT | S1822 | 40.296 | 29.386 | 23.361 | 1.00 | 44.10 | S |
| ATOM | 3019 | OH2 | WAT | S1823 | 42.915 | 30.163 | 27.417 | 1.00 | 33.23 | S |
| ATOM | 3020 | OH2 | WAT | S1824 | 14.322 | 38.428 | 8.032  | 1.00 | 35.73 | S |
| ATOM | 3021 | OH2 | WAT | S1825 | 33.329 | 16.000 | 45.385 | 1.00 | 29.78 | S |
| ATOM | 3022 | OH2 | WAT | S1826 | 55.683 | 28.168 | 38.449 | 1.00 | 30.81 | S |
| ATOM | 3023 | OH2 | WAT | S1827 | 18.514 | 45.706 | 9.695  | 1.00 | 34.33 | S |
| ATOM | 3024 | OH2 | WAT | S1828 | 19.453 | 54.788 | 22.809 | 1.00 | 42.02 | S |
| ATOM | 3025 | OH2 | WAT | S1829 | 46.686 | 27.005 | 20.816 | 1.00 | 31.17 | S |
| ATOM | 3026 | OH2 | WAT | S1830 | 50.779 | 32.327 | 54.666 | 1.00 | 44.04 | S |
| ATOM | 3027 | OH2 | WAT | S1831 | 5.243  | 43.614 | 40.262 | 1.00 | 40.69 | S |
| ATOM | 3028 | OH2 | WAT | S1832 | 45.151 | 43.041 | 33.919 | 1.00 | 28.47 | S |
| ATOM | 3029 | OH2 | WAT | S1833 | 26.385 | 11.949 | 41.104 | 1.00 | 33.70 | S |
| ATOM | 3030 | OH2 | WAT | S1834 | 36.104 | 26.756 | 17.653 | 1.00 | 32.43 | S |
| ATOM | 3031 | OH2 | WAT | S1835 | 40.585 | 7.298  | 41.894 | 1.00 | 32.97 | S |
| ATOM | 3032 | OH2 | WAT | S1836 | 22.940 | 54.196 | 16.985 | 1.00 | 39.88 | S |
| ATOM | 3033 | OH2 | WAT | S1837 | 53.968 | 24.450 | 37.442 | 1.00 | 39.29 | S |
| ATOM | 3034 | OH2 | WAT | S1838 | 16.318 | 26.973 | 42.179 | 1.00 | 32.94 | S |
| ATOM | 3035 | OH2 | WAT | S1839 | 14.513 | 48.940 | 39.307 | 1.00 | 29.97 | S |

FIGURE 5 (suite)

|      |      |     |     |       |        |        |        |      |       |   |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|---|
| ATOM | 3036 | OH2 | WAT | S1840 | 31.652 | 6.945  | 51.493 | 1.00 | 27.66 | S |
| ATOM | 3037 | OH2 | WAT | S1841 | 41.996 | 11.677 | 38.039 | 1.00 | 37.88 | S |
| ATOM | 3038 | OH2 | WAT | S1842 | 7.510  | 48.642 | 19.668 | 1.00 | 35.11 | S |
| ATOM | 3039 | OH2 | WAT | S1843 | 42.467 | 3.493  | 49.912 | 1.00 | 33.41 | S |
| ATOM | 3040 | OH2 | WAT | S1844 | 59.776 | 22.501 | 42.412 | 1.00 | 44.37 | S |
| ATOM | 3041 | OH2 | WAT | S1845 | 7.867  | 44.473 | 12.687 | 1.00 | 34.20 | S |
| ATOM | 3042 | OH2 | WAT | S1846 | 15.405 | 45.353 | 39.658 | 1.00 | 38.08 | S |
| ATOM | 3043 | OH2 | WAT | S1847 | 13.585 | 15.183 | 28.501 | 1.00 | 36.58 | S |
| ATOM | 3044 | OH2 | WAT | S1848 | 48.442 | 41.492 | 47.985 | 1.00 | 26.95 | S |
| ATOM | 3045 | OH2 | WAT | S1849 | 50.374 | 40.886 | 46.017 | 1.00 | 34.93 | S |
| ATOM | 3046 | OH2 | WAT | S1850 | 44.568 | 8.030  | 45.822 | 1.00 | 42.34 | S |
| ATOM | 3047 | OH2 | WAT | S1851 | 48.705 | 28.443 | 22.632 | 1.00 | 34.87 | S |
| ATOM | 3048 | OH2 | WAT | S1852 | 38.217 | 33.408 | 18.268 | 1.00 | 40.91 | S |
| ATOM | 3049 | OH2 | WAT | S1853 | 26.698 | 47.866 | 16.749 | 1.00 | 26.87 | S |
| ATOM | 3050 | OH2 | WAT | S1854 | 36.624 | 40.405 | 57.361 | 1.00 | 30.57 | S |
| ATOM | 3051 | OH2 | WAT | S1855 | 44.243 | 22.209 | 21.682 | 1.00 | 25.97 | S |
| ATOM | 3052 | OH2 | WAT | S1856 | 50.807 | 22.291 | 30.826 | 1.00 | 30.01 | S |
| ATOM | 3053 | OH2 | WAT | S1857 | 2.113  | 19.175 | 16.420 | 1.00 | 39.64 | S |
| ATOM | 3054 | OH2 | WAT | S1858 | 35.799 | 20.261 | 25.717 | 1.00 | 29.95 | S |
| ATOM | 3055 | OH2 | WAT | S1859 | 10.845 | 51.013 | 18.474 | 1.00 | 29.30 | S |
| ATOM | 3056 | OH2 | WAT | S1860 | 13.036 | 16.982 | 18.603 | 1.00 | 35.56 | S |
| ATOM | 3057 | OH2 | WAT | S1861 | 48.755 | 33.466 | 53.529 | 1.00 | 32.19 | S |
| ATOM | 3058 | OH2 | WAT | S1862 | 28.542 | 12.640 | 28.777 | 1.00 | 32.37 | S |
| ATOM | 3059 | OH2 | WAT | S1863 | 15.582 | 33.781 | 40.294 | 1.00 | 31.38 | S |
| ATOM | 3060 | OH2 | WAT | S1864 | 15.389 | 51.736 | 31.264 | 1.00 | 35.97 | S |
| ATOM | 3061 | OH2 | WAT | S1865 | 59.586 | 24.576 | 44.154 | 1.00 | 38.45 | S |
| ATOM | 3062 | OH2 | WAT | S1866 | 33.931 | 18.197 | 52.470 | 1.00 | 31.45 | S |
| ATOM | 3063 | OH2 | WAT | S1867 | 33.400 | 24.810 | 14.487 | 1.00 | 31.43 | S |
| ATOM | 3064 | OH2 | WAT | S1868 | 2.939  | 39.474 | 28.464 | 1.00 | 42.13 | S |
| ATOM | 3065 | OH2 | WAT | S1869 | 52.149 | 36.661 | 45.439 | 1.00 | 34.90 | S |
| ATOM | 3066 | OH2 | WAT | S1870 | 45.901 | 34.119 | 54.146 | 1.00 | 28.55 | S |
| ATOM | 3067 | OH2 | WAT | S1871 | 21.485 | 29.372 | 44.666 | 1.00 | 37.03 | S |
| ATOM | 3068 | OH2 | WAT | S1872 | 10.455 | 19.175 | 23.705 | 1.00 | 36.18 | S |
| ATOM | 3069 | OH2 | WAT | S1873 | 29.820 | 54.141 | 17.625 | 1.00 | 37.56 | S |
| ATOM | 3070 | OH2 | WAT | S1874 | 36.824 | 12.036 | 41.616 | 1.00 | 36.62 | S |
| ATOM | 3071 | OH2 | WAT | S1875 | 35.575 | 29.695 | 13.582 | 1.00 | 31.58 | S |
| ATOM | 3072 | OH2 | WAT | S1876 | 47.689 | 26.645 | 56.483 | 1.00 | 29.75 | S |
| ATOM | 3073 | OH2 | WAT | S1877 | 25.923 | 24.021 | 7.877  | 1.00 | 35.32 | S |
| ATOM | 3074 | OH2 | WAT | S1878 | 35.914 | 42.663 | 19.444 | 1.00 | 38.13 | S |
| ATOM | 3075 | OH2 | WAT | S1879 | 53.553 | 27.199 | 37.462 | 1.00 | 34.02 | S |
| ATOM | 3076 | OH2 | WAT | S1880 | 31.012 | 18.989 | 51.960 | 1.00 | 32.14 | S |
| ATOM | 3077 | OH2 | WAT | S1881 | 5.543  | 24.207 | 39.126 | 1.00 | 33.92 | S |
| ATOM | 3078 | OH2 | WAT | S1882 | 12.515 | 49.450 | 14.280 | 1.00 | 38.32 | S |
| ATOM | 3079 | OH2 | WAT | S1883 | 19.621 | 34.441 | 42.264 | 1.00 | 32.10 | S |
| ATOM | 3080 | OH2 | WAT | S1884 | 0.567  | 34.443 | 15.606 | 1.00 | 41.76 | S |
| ATOM | 3081 | OH2 | WAT | S1885 | 19.842 | 21.597 | 48.228 | 1.00 | 38.20 | S |
| ATOM | 3082 | OH2 | WAT | S1886 | 17.245 | 44.489 | 41.443 | 1.00 | 36.34 | S |
| ATOM | 3083 | OH2 | WAT | S1887 | 31.241 | 17.703 | 18.315 | 1.00 | 43.85 | S |
| ATOM | 3084 | OH2 | WAT | S1888 | 47.120 | 35.974 | 31.511 | 1.00 | 44.95 | S |
| ATOM | 3085 | OH2 | WAT | S1889 | 16.721 | 12.447 | 25.646 | 1.00 | 42.81 | S |
| ATOM | 3086 | OH2 | WAT | S1890 | 17.002 | 21.309 | 47.530 | 1.00 | 35.74 | S |
| ATOM | 3087 | OH2 | WAT | S1891 | 11.124 | 36.224 | 11.415 | 1.00 | 28.23 | S |
| ATOM | 3088 | OH2 | WAT | S1892 | 31.476 | 35.439 | 12.666 | 1.00 | 29.98 | S |
| ATOM | 3089 | OH2 | WAT | S1893 | 20.313 | 44.798 | 8.239  | 1.00 | 38.49 | S |
| ATOM | 3090 | OH2 | WAT | S1894 | 49.492 | 37.692 | 31.490 | 1.00 | 34.21 | S |
| ATOM | 3091 | OH2 | WAT | S1895 | 11.168 | 48.631 | 11.775 | 1.00 | 35.00 | S |
| ATOM | 3092 | OH2 | WAT | S1896 | 8.149  | 35.174 | 12.830 | 1.00 | 43.18 | S |
| ATOM | 3093 | OH2 | WAT | S1897 | 42.985 | 36.028 | 29.277 | 1.00 | 37.84 | S |
| ATOM | 3094 | OH2 | WAT | S1898 | 15.722 | 26.088 | 38.269 | 1.00 | 40.56 | S |
| ATOM | 3095 | OH2 | WAT | S1899 | 9.466  | 42.584 | 43.325 | 1.00 | 38.58 | S |
| ATOM | 3096 | OH2 | WAT | S1900 | 55.683 | 27.859 | 55.011 | 1.00 | 40.16 | S |
| ATOM | 3097 | OH2 | WAT | S1901 | 16.412 | 44.824 | 6.088  | 1.00 | 35.00 | S |
| ATOM | 3098 | OH2 | WAT | S1902 | 30.819 | 20.863 | 13.376 | 1.00 | 36.12 | S |
| ATOM | 3099 | OH2 | WAT | S1903 | 20.083 | 45.050 | 40.249 | 1.00 | 46.55 | S |
| ATOM | 3100 | OH2 | WAT | S1904 | 55.216 | 16.767 | 37.256 | 1.00 | 32.34 | S |
| ATOM | 3101 | OH2 | WAT | S1905 | 17.194 | 15.633 | 31.289 | 1.00 | 41.92 | S |
| ATOM | 3102 | OH2 | WAT | S1906 | 55.468 | 39.305 | 45.956 | 1.00 | 33.48 | S |
| ATOM | 3103 | OH2 | WAT | S1907 | 34.073 | 59.171 | 22.880 | 1.00 | 29.68 | S |
| ATOM | 3104 | OH2 | WAT | S1908 | 11.696 | 23.487 | 37.533 | 1.00 | 44.83 | S |
| ATOM | 3105 | OH2 | WAT | S1909 | 37.193 | 57.700 | 24.645 | 1.00 | 29.20 | S |
| ATOM | 3106 | OH2 | WAT | S1910 | 4.958  | 20.071 | 12.971 | 1.00 | 38.75 | S |
| ATOM | 3107 | OH2 | WAT | S1911 | 28.212 | 15.651 | 46.090 | 1.00 | 44.28 | S |
| ATOM | 3108 | OH2 | WAT | S1912 | 25.791 | 17.881 | 50.101 | 1.00 | 44.07 | S |
| ATOM | 3109 | OH2 | WAT | S1913 | 44.830 | 16.225 | 28.015 | 1.00 | 37.34 | S |
| ATOM | 3110 | OH2 | WAT | S1914 | 45.538 | 25.603 | 58.524 | 1.00 | 31.60 | S |
| ATOM | 3111 | OH2 | WAT | S1915 | 31.849 | 53.832 | 20.135 | 1.00 | 44.08 | S |

FIGURE 5 (suite)

|      |      |     |     |       |        |        |        |      |       |   |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|---|
| ATOM | 3112 | OH2 | WAT | S1916 | 55.981 | 32.376 | 47.108 | 1.00 | 41.65 | S |
| ATOM | 3113 | OH2 | WAT | S1917 | 35.699 | 24.353 | 16.736 | 1.00 | 43.04 | S |
| ATOM | 3114 | OH2 | WAT | S1918 | 3.252  | 25.157 | 38.490 | 1.00 | 42.38 | S |
| ATOM | 3115 | OH2 | WAT | S1919 | 34.711 | 10.496 | 39.861 | 1.00 | 36.97 | S |
| ATOM | 3116 | OS4 | PLA | P1001 | 8.781  | 29.613 | 10.689 | 1.00 | 35.34 | P |
| ATOM | 3117 | S2  | PLA | P1001 | 9.783  | 28.546 | 11.256 | 1.00 | 33.57 | P |
| ATOM | 3118 | OS5 | PLA | P1001 | 10.409 | 27.663 | 9.867  | 1.00 | 40.37 | P |
| ATOM | 3119 | OS6 | PLA | P1001 | 11.159 | 29.189 | 12.135 | 1.00 | 41.03 | P |
| ATOM | 3120 | C15 | PLA | P1001 | 9.058  | 27.351 | 12.199 | 1.00 | 30.49 | P |
| ATOM | 3121 | C14 | PLA | P1001 | 7.662  | 27.126 | 12.015 | 1.00 | 23.35 | P |
| ATOM | 3122 | C16 | PLA | P1001 | 9.978  | 26.532 | 12.898 | 1.00 | 28.94 | P |
| ATOM | 3123 | C10 | PLA | P1001 | 9.499  | 25.436 | 13.634 | 1.00 | 30.90 | P |
| ATOM | 3124 | C11 | PLA | P1001 | 8.025  | 25.127 | 13.485 | 1.00 | 25.22 | P |
| ATOM | 3125 | C13 | PLA | P1001 | 7.134  | 25.968 | 12.614 | 1.00 | 21.41 | P |
| ATOM | 3126 | O3  | PLA | P1001 | 5.837  | 25.588 | 12.437 | 1.00 | 24.00 | P |
| ATOM | 3127 | C12 | PLA | P1001 | 7.519  | 23.932 | 14.212 | 1.00 | 27.53 | P |
| ATOM | 3128 | O2  | PLA | P1001 | 6.235  | 23.585 | 13.967 | 1.00 | 21.97 | P |
| ATOM | 3129 | C9  | PLA | P1001 | 10.366 | 24.618 | 14.415 | 1.00 | 32.13 | P |
| ATOM | 3130 | C8  | PLA | P1001 | 9.876  | 23.541 | 15.205 | 1.00 | 31.56 | P |
| ATOM | 3131 | S1  | PLA | P1001 | 10.846 | 22.324 | 15.981 | 1.00 | 31.16 | P |
| ATOM | 3132 | OS3 | PLA | P1001 | 12.358 | 22.881 | 16.679 | 1.00 | 39.44 | P |
| ATOM | 3133 | OS2 | PLA | P1001 | 11.138 | 21.153 | 14.733 | 1.00 | 28.72 | P |
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| ATOM | 3135 | C7  | PLA | P1001 | 8.424  | 23.154 | 15.086 | 1.00 | 20.93 | P |
| ATOM | 3136 | N2  | PLA | P1001 | 7.947  | 21.974 | 15.652 | 1.00 | 27.49 | P |
| ATOM | 3137 | N1  | PLA | P1001 | 6.731  | 21.270 | 15.708 | 1.00 | 26.74 | P |
| ATOM | 3138 | C2  | PLA | P1001 | 6.780  | 19.948 | 16.206 | 1.00 | 29.90 | P |
| ATOM | 3139 | C1  | PLA | P1001 | 7.938  | 19.230 | 16.659 | 1.00 | 26.11 | P |
| ATOM | 3140 | C3  | PLA | P1001 | 5.455  | 19.218 | 16.215 | 1.00 | 29.97 | P |
| ATOM | 3141 | O1  | PLA | P1001 | 4.329  | 19.881 | 15.839 | 1.00 | 27.77 | P |
| ATOM | 3142 | C4  | PLA | P1001 | 5.419  | 17.867 | 16.622 | 1.00 | 27.79 | P |
| ATOM | 3143 | C5  | PLA | P1001 | 6.617  | 17.226 | 17.060 | 1.00 | 24.04 | P |
| ATOM | 3144 | C6  | PLA | P1001 | 7.890  | 17.875 | 17.105 | 1.00 | 28.93 | P |
| ATOM | 3145 | CL1 | PLA | P1001 | 8.958  | 17.179 | 17.619 | 1.00 | 13.83 | P |
| ATOM | 3146 | OS4 | PLA | P1002 | -1.265 | 32.010 | 14.293 | 1.00 | 40.73 | P |
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| ATOM | 3148 | OS5 | PLA | P1002 | -3.293 | 32.318 | 16.225 | 1.00 | 36.70 | P |
| ATOM | 3149 | OS6 | PLA | P1002 | -3.702 | 31.417 | 13.545 | 1.00 | 38.28 | P |
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| ATOM | 3151 | C14 | PLA | P1002 | -1.339 | 29.023 | 14.693 | 1.00 | 32.35 | P |
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| ATOM | 3155 | C13 | PLA | P1002 | -1.219 | 27.623 | 14.849 | 1.00 | 32.76 | P |
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| ATOM | 3157 | C12 | PLA | P1002 | -2.103 | 25.533 | 16.170 | 1.00 | 29.76 | P |
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| ATOM | 3159 | C9  | PLA | P1002 | -4.076 | 27.177 | 17.503 | 1.00 | 28.28 | P |
| ATOM | 3160 | C8  | PLA | P1002 | -4.072 | 25.777 | 17.756 | 1.00 | 30.57 | P |
| ATOM | 3161 | S1  | PLA | P1002 | -4.937 | 25.049 | 19.065 | 1.00 | 30.09 | P |
| ATOM | 3162 | OS3 | PLA | P1002 | -6.417 | 25.925 | 19.382 | 1.00 | 26.32 | P |
| ATOM | 3163 | OS2 | PLA | P1002 | -3.886 | 25.328 | 20.444 | 1.00 | 39.20 | P |
| ATOM | 3164 | OS1 | PLA | P1002 | -5.060 | 23.483 | 18.960 | 1.00 | 35.43 | P |
| ATOM | 3165 | C7  | PLA | P1002 | -3.056 | 24.884 | 17.116 | 1.00 | 30.01 | P |
| ATOM | 3166 | N2  | PLA | P1002 | -2.942 | 23.547 | 17.510 | 1.00 | 30.83 | P |
| ATOM | 3167 | N1  | PLA | P1002 | -1.994 | 22.600 | 17.132 | 1.00 | 26.11 | P |
| ATOM | 3168 | C2  | PLA | P1002 | -2.109 | 21.347 | 17.777 | 1.00 | 33.57 | P |
| ATOM | 3169 | C1  | PLA | P1002 | -3.069 | 20.979 | 18.767 | 1.00 | 28.55 | P |
| ATOM | 3170 | C3  | PLA | P1002 | -1.126 | 20.289 | 17.352 | 1.00 | 32.70 | P |
| ATOM | 3171 | O1  | PLA | P1002 | -0.254 | 20.633 | 16.366 | 1.00 | 26.71 | P |
| ATOM | 3172 | C4  | PLA | P1002 | -1.181 | 19.011 | 17.978 | 1.00 | 35.63 | P |
| ATOM | 3173 | C5  | PLA | P1002 | -2.175 | 18.727 | 18.965 | 1.00 | 32.99 | P |
| ATOM | 3174 | C6  | PLA | P1002 | -3.137 | 19.696 | 19.364 | 1.00 | 34.82 | P |
| ATOM | 3175 | CL1 | PLA | P1002 | -4.110 | 19.418 | 20.286 | 1.00 | 26.50 | P |
| ATOM | 3176 | P   | PO4 | I1000 | 31.378 | 36.578 | 34.442 | 1.00 | 7.30  | I |
| ATOM | 3177 | O1  | PO4 | I1000 | 30.121 | 37.237 | 34.900 | 1.00 | 8.97  | I |
| ATOM | 3178 | O2  | PO4 | I1000 | 32.276 | 37.563 | 33.795 | 1.00 | 6.24  | I |
| ATOM | 3179 | O3  | PO4 | I1000 | 31.043 | 35.497 | 33.462 | 1.00 | 6.45  | I |
| ATOM | 3180 | O4  | PO4 | I1000 | 32.089 | 35.965 | 35.624 | 1.00 | 7.79  | I |
| ATOM | 3181 | U   | U   | I1100 | 0.273  | 22.910 | 15.547 | 1.00 | 30.28 | I |
| ATOM | 3182 | U   | U   | I1101 | 4.450  | 22.112 | 14.520 | 1.00 | 29.14 | I |
| ATOM | 3183 | U   | U   | I1102 | 2.292  | 24.635 | 12.979 | 0.50 | 39.41 | I |
| ATOM | 3184 | NA  | NA  | I1200 | 37.019 | 13.768 | 54.963 | 1.00 | 21.53 | I |
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FIGURE 5 (suite)

## LISTE DE SEQUENCES

<110> CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE  
UNIVERSITE HENRI POINCARÉ DE NANCY

<120> NOUVELLE PROTEINE DE LIAISON AU PHOSPHATE, COMPOSITIONS  
PHARMACEUTIQUES LA CONTENANT ET SES UTILISATIONS

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# INTERNATIONAL SEARCH REPORT

International Application No  
/FR2004/002797

A. CLASSIFICATION OF SUBJECT MATTER  
IPC 7 C07K14/47

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)  
IPC 7 C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, Sequence Search, BIOSIS, EMBASE, PAJ, WPI Data

C. DOCUMENTS CONSIDERED TO BE RELEVANT

| Category * | Citation of document, with indication, where appropriate, of the relevant passages  | Relevant to claim No. |
|------------|---|-----------------------|
| X          | US 2003/158115 A1 (LIESKE JOHN C ET AL)<br>21 August 2003 (2003-08-21)<br>abstract<br>example 6<br>SEQ ID No 16<br>-----<br>DATABASE UNIPROT 'Online'<br>EBI; 10 October 2003 (2003-10-10),<br>XP002275669<br>Database accession no. P35482<br>the whole document<br>-----<br>-/- | 1-9                   |
| X          |   | 1-9                   |

Further documents are listed in the continuation of box C.

Patent family members are listed in annex.

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- \*A\* document defining the general state of the art which is not considered to be of particular relevance
- \*E\* earlier document but published on or after the international filing date
- \*L\* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
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Date of the actual completion of the international search

23 March 2005

Date of mailing of the international search report

01/04/2005

Name and mailing address of the ISA

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**INTERNATIONAL SEARCH REPORT**

Information on patent family members

International Application No

/FR2004/002797

| Patent document cited in search report | Publication date | Patent family member(s) | Publication date |
|--|------------------|-------------------------|------------------|
| US 2003158115                          | A1 21-08-2003    | US 6482934 B1           | 19-11-2002       |

# RAPPORT DE RECHERCHE INTERNATIONALE

Recherche internationale No  
/FR2004/002797

A. CLASSEMENT DE L'OBJET DE LA DEMANDE  
CIB 7 C07K14/47

Selon la classification internationale des brevets (CIB) ou à la fois selon la classification nationale et la CIB

## B. DOMAINES SUR LESQUELS LA RECHERCHE A PORTE

Documentation minimale consultée (système de classification suivi des symboles de classement)  
CIB 7 C07K

Documentation consultée autre que la documentation minimale dans la mesure où ces documents relèvent des domaines sur lesquels a porté la recherche

Base de données électronique consultée au cours de la recherche internationale (nom de la base de données, et si réalisable, termes de recherche utilisés)  
EPO-Internal, Sequence Search, BIOSIS, EMBASE, PAJ, WPI Data

## C. DOCUMENTS CONSIDERES COMME PERTINENTS

| Catégorie | Identification des documents cités, avec, le cas échéant, l'indication des passages pertinents   | no. des revendications visées |
|-----------|--|-------------------------------|
| X         | US 2003/158115 A1 (LIESKE JOHN C ET AL)<br>21 août 2003 (2003-08-21)<br>abrégé<br>exemple 6<br>SEQ ID No 16<br>-----<br>DATABASE UNIPROT 'Online'<br>EBI; 10 octobre 2003 (2003-10-10),<br>XP002275669<br>Database accession no. P35482<br>1e document en entier<br>-----<br>-/- | 1-9                           |
| X         |  | 1-9                           |

Voir la suite du cadre C pour la fin de la liste des documents

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Date à laquelle la recherche internationale a été effectivement achevée

23 mars 2005

Date d'expédition du présent rapport de recherche internationale

01/04/2005

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Fonctionnaire autorisé

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**RAPPORT DE RECHERCHE INTERNATIONALE**

Renseignements rel

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Rapport de recherche internationale No

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| Document brevet cité<br>au rapport de recherche | Date de<br>publication | Membre(s) de la<br>famille de brevet(s) | Date de<br>publication |
|---|------------------------|---|------------------------|
| US 2003158115                                   | A1 21-08-2003          | US 6482934 B1                           | 19-11-2002             |